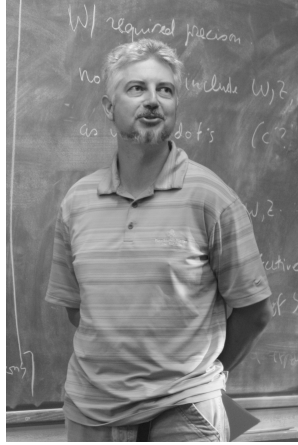# Flavor physics and lattice quantum chromodynamics

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To Annemarie, Benjamin and Niels

Acknowledgements

Preface

Quark flavor physics and lattice quantum chromodynamics (QCD) met many years ago, and together have given rise to a vast number of very fruitful studies. All of these studies certainly cannot be reviewed within the course of these lectures. Instead of attempting to do so, I discuss in some detail the fascinating theoretical and phenomenological context and background behind them, and use the rich phenomenology of nonleptonic weak kaon decays as a template to present some key techniques and to show how lattice QCD can effectively help shed light on these important phenomena. Even though the lattice study of $K \to \pi\pi$ decays originated in the mid-eighties, it is still highly relevant. In particular, testing the consistency of the Standard Model with the beautiful experimental measurements of direct CP violation in these decays remains an important goal for the upcoming generation of lattice QCD practitioners.

The course begins with an introduction to the Standard Model, viewed as an effective field theory. Experimental and theoretical limits on the energy scales at which New Physics can appear, as well as current constraints on quark flavor parameters, are reviewed. The role of lattice QCD in obtaining these constraints is described. A second section is devoted to explaining the Cabibbo-Kobayashi-Maskawa mechanism for quark flavor mixing and CP violation, and to detailing its most salient features. The third section is dedicated to the study of $K \to \pi\pi$ decays. It comprises discussions of indirect CP violation through K^0-$\bar{K}^0$ mixing, of the $\Delta I = 1/2$ rule and of direct CP violation. It presents some of the lattice QCD tools required to describe these phenomena *ab initio.*

Contents

1
Introduction and motivation

1.1   The Standard Model as a low-energy effective field theory

If elementary particles were massless, their fundamental interactions would be well described by the most general perturbatively renormalizable [1] relativistic quantum field theory based on:

- the gauge group
$$SU(3)_c \times SU(2)_L \times U(1)_Y \ , \tag{1.1}$$
  where the subscript c stands for "color", L for left-handed weak isospin and Y for hypercharge;
- three families of quarks and leptons
$$\begin{cases} u \ d \ e^- \ \nu_e \\ c \ s \ \mu^- \ \nu_\mu \\ t \ b \ \tau^- \ \nu_\tau \end{cases} \ , \tag{1.2}$$
  with prescribed couplings to the gauge fields (i.e. in specific representations of the gauge groups);
- and the absence of anomalies.

In the presence of masses for the weak gauge bosons $W^\pm$ and Z^0, for the quarks and for the leptons, the most economical way known to keep this construction perturbatively renormalizable is to implement the Higgs mechanism (Englert and Brout, 1964; Higgs, 1964), as done in the Standard Model (SM). However, this results in adding a yet unobserved degree of freedom to the model, the Higgs boson.

By calling a theory renormalizable we mean that it can be used to make *predictions of arbitrarily high accuracy* over a very large interval of energies, ranging from zero to possibly infinite energy, with only a finite number of coupling constants. [2] These couplings are associated with operators of mass dimension less or equal to four in $3+1$ dimensions.

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[1] Beyond fixed-order perturbation theory, the $U(1)_Y$ of hypercharge is *trivial:* the renormalized coupling constant vanishes when the cutoff of the regularized theory is taken to infinity, a notion first suggested in (Wilson and Kogut, 1974).

[2] If one sticks to perturbation theory, the precision reached is actually limited by the fact that perturbative expansions in field theory are typically asymptotic expansions. Moreover, the triviality of the Higgs and $U(1)_Y$ sectors means that the cutoff, which we generically call Λ here, has to be kept finite. This limits the accuracy of predictions through the presence of regularization dependent corrections which are proportional to powers of E/Λ, where E is an energy typical of the process studied. In that sense, only asymptotically free theories can be fundamental since they are the only ones that can be used to describe phenomena up to arbitrarily high energies.

Renormalizable field theories are remarkable in many ways. Consider an arbitrary high-energy theory described by a Lagrangian $\mathcal{L}_{\mathrm{UV}}$ (e.g. a GUT, a string theory, ...) with given low-energy spectrum and symmetries. At sufficiently low energies this theory is described by the unique renormalizable theory with the given spectrum and symmetries, whose Lagrangian we will denote $\mathcal{L}_{\mathrm{ren}}$. Moreover, the deviations between the predictions of the two theories can be parametrized through a local low-energy effective field theory (EFT)

$$\mathcal{L}_{\mathrm{UV}} = \mathcal{L}_{\mathrm{ren}} + \sum_{d \geq 4} \sum_i \frac{C_{d,i}}{\Lambda_i^{d-4}} O_i^{(d)} \ , \tag{1.3}$$

where the $O_i^{(d)}$ are operators of mass dimension $d \geq 4$ built up from fields of $\mathcal{L}_{\mathrm{ren}}$. The Λ_i are mass scales which are much larger than the masses in the spectrum of $\mathcal{L}_{\mathrm{ren}}$– there may be one or many of them depending on the number of distinct scales in $\mathcal{L}_{\mathrm{UV}}$. The $C_{d,i}$ are dimensionless coefficients whose sizes depend on how the corresponding operators are generated in the UV theory, e.g. at tree or loop level.

Thus, very generally, we can write down the Lagrangian of particle physics as a low-energy EFT with the gauge group of Eq. (1.1), the matter content of Eq. (1.2) and a Higgs mechanism:

$$\mathcal{L}_{\mathrm{SM}}^{\mathrm{eff}} = \mathcal{L}_{\mathrm{SM}} + \frac{1}{M} O_{\mathrm{Maj}}^{(5)} + \sum_{d \geq 6} \sum_i \frac{C_{d,i}}{\Lambda_i^{d-4}} O_i^{(d)} \ , \tag{1.4}$$

where the left-handed neutrino Majorana mass term, $O_{\mathrm{Maj}}^{(5)}$, and the $O_i^{(d)}$ must be invariant under the Standard Model gauge group (1.1). In Eq. (1.4), $\mathcal{L}_{\mathrm{SM}}$ is the renormalizable Standard Model Lagrangian

$$\mathcal{L}_{\mathrm{SM}} = \mathcal{L}_{\mathrm{g+f}} + \mathcal{L}_{\mathrm{flavor}} + \mathcal{L}_{\mathrm{EWSB}} + \mathcal{L}_\nu \ . \tag{1.5}$$

where $\mathcal{L}_{\mathrm{g+f}}$ contains the gauge and fermion kinetic and coupling terms, $\mathcal{L}_{\mathrm{flavor}}$, the Higgs-Yukawa terms, $\mathcal{L}_{\mathrm{EWSB}}$, the Higgs terms and $\mathcal{L}_\nu$, the possible renormalizable neutrino mass and right-handed neutrino kinetic terms. In that sense, the renormalizable Standard Model is a low-energy approximation of a more complete high-energy theory involving scales of New Physics much larger than M_W.

Schematically, the gauge and fermion Lagrangian reads

$$\mathcal{L}_{\mathrm{g+f}} = \frac{1}{4} F_{\mu\nu}^a F_a^{\mu\nu} + \bar{\psi} \slashed{D} \psi \ . \tag{1.6}$$

It has 3 parameters, the gauge couplings (g_1, g_2, g_3), and is very well tested through experiments conducted at LEP, SLC, the Tevatron, etc. Its parameters are known to better than per mil accuracy.

The Higgs-Yukawa terms are given by

$$\mathcal{L}_{\mathrm{flavor}} = -\bar{\psi}_R^{(-1/2)} Y_{(-1/2)} \phi^\dagger \psi_L - \bar{\psi}_R^{(1/2)} Y_{(1/2)} \tilde{\phi}^\dagger \psi_L + \mathrm{h.c.} \ , \tag{1.7}$$

with ψ_L corresponding to the left-handed $SU(2)_L$ doublets and $\psi_R^{(\pm 1/2)}$ the right-handed $SU(2)_L$ singlets, associated with the $I_3 = \pm\frac{1}{2}$ component of the doublets.

In this equation, ϕ is the Higgs field and $\tilde{\phi}$ its conjugate, $(\phi^0, -\phi^{+*})$. The flavor component of the Standard Model Lagrangian has many more couplings, 13 in fact. It gives rise to the 3 charged lepton masses, 6 quark masses and the quark flavor mixing matrix which has 3 mixing angles and 1 phase. [3] The understanding of this quark mixing and its associated CP violation will be the main focus of the present course.

There is also the electroweak symmetry breaking (EWSB) contribution

$$\mathcal{L}_{\text{EWSB}} = (D_\mu \phi)^\dagger (D^\mu \phi) - \mu^2 \phi^\dagger \phi - \lambda (\phi^\dagger \phi)^2 \ . \tag{1.8}$$

It has only 2 couplings, the Higgs mass and self-coupling (μ, λ), and is very poorly tested so far, a situation which will change radically with the LHC.

As for the neutrino Lagrangian, little is known from experiment about its form. There are theoretically two possible, nonexclusive scenarios:

1. There are no right-handed neutrinos in sight. Thus, we give our left-handed neutrinos a mass without introducing a right-handed partner. In that case, $\mathcal{L}_\nu = 0$ in Eq. (1.5) and we have a Majorana mass term for the left-handed neutrinos in Eq. (1.4), with

$$O_{\text{Maj}}^{(5)} = -\frac{1}{2} \nu_L^T C \tilde{\phi}^T A_\nu^L \tilde{\phi} \nu_L + \text{h.c.} \ , \tag{1.9}$$

   where C is the charge conjugation matrix (see Eq. (2.22)). That is, after EWSB the neutrino acquire a Majorana mass through the introduction of a nonrenormalizable dimension-5 operator. This implies that the Standard Model is an EFT and that we already have a signal for a new mass scale. Indeed, with $m_\nu \sim 0.1$ eV (a plausible value), eigenvalues of the coupling matrix A_ν^L of order 1 and $\langle \phi \rangle \sim 246$ GeV, one finds for the mass scale M of Eq. (1.4)

$$M \sim \frac{\langle \phi \rangle^2}{m_\nu} \sim 10^{15} \, \text{GeV} \tag{1.10}$$

   which is tantalizingly close to a possible unification scale.

2. We choose to allow right-handed neutrinos, N_R. These neutrinos must be singlets under the Standard Model group. Thus, they themselves may have a Majorana mass, but this time a renormalizable one, in addition to allowing the presence of a Dirac mass term:

$$\mathcal{L}_\nu = N_R i \displaystyle{\not{\partial}} N_R - (\bar{L}_L Y_\nu^\dagger \tilde{\phi} N_R + \frac{1}{2} N_R^T C M_\nu^R N_R + \text{h.c.}) \tag{1.11}$$

$$= N_R i \displaystyle{\not{\partial}} N_R - \frac{1}{2} (\nu_L^T, N_R^{cT}) C \begin{pmatrix} 0 & Y_\nu^\dagger \phi^0 \\ Y_\nu^* \phi^0 & M_\nu^R \end{pmatrix} \begin{pmatrix} \nu_L \\ N_R^c \end{pmatrix} + \cdots \ , \tag{1.12}$$

   where L_L stands for the left-handed lepton doublets, and N_R^c for the charge conjugate of N_R (see Eq. (2.22)).

   There are here three more possibilities:

   a) $M_\nu^R = 0$

   In that case, the three neutrinos have Dirac masses and lepton number is conserved.

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[3] Remember that we have separated out into $\mathcal{L}_\nu$ possible renormalizable neutrino mass terms.

b) $M_\nu^R \gg Y_\nu \langle \phi \rangle$

Here, the see-saw mechanism comes into play: there are no right-handed neutrinos in sight and all three left-handed neutrinos acquire a mass through $d = 5$ operators:

$$\mathcal{L}_{\text{eff}}^{m_\nu} = -\frac{1}{2} \nu_L^T C \tilde{\phi}^T \left(Y_\nu^\dagger (M_\nu^R)^{-1} Y_\nu^* \right) \tilde{\phi} \nu_L + O\left((M_\nu^R)^{-2} \right) \ . \tag{1.13}$$

Thus, we have an explicit realization of scenario 1).
Taking $\text{Re} Y_\nu \langle \phi \rangle \sim 1\,\text{GeV}$ in rough analogy with the τ and again, $m_\nu \sim 0.1\,\text{eV}$, we obtain for the mass scale M of Eq. (1.4)

$$M \sim \frac{(\text{Re} Y_\nu \langle \phi \rangle)^2}{m_\nu} \sim 10^{10}\,\text{GeV} \ . \tag{1.14}$$

c) Some eigenvalues of $M \sim$ some eigenvalues of $Y_\nu \langle \phi \rangle$

Then, the sea-saw neutrino mass matrix will have more than three small distinct eigenvalues (actually up to six), leading to more than three light neutrinos. Such a possibility is constrained by phenomenology, but is not excluded.

Though the topic of neutrino masses and associated mixing and CP violation is fascinating, it is not the flavor physics which is of interest to us here. Thus, this is all that we will say about the subject and, for the remainder of the course, we can safely take $m_\nu = 0$, forgetting about $O_{\text{Maj}}^{(5)}$ and $\mathcal{L}_\nu$ altogether.

Having explored the neutrino mass Lagrangian and some of the constraints which neutrinos place on the scale of New Physics, we now do the same for the other components of $\mathcal{L}_{\text{SM}}^{\text{eff}}$, generically denoting the scale of New Physics by Λ:

1. *EWSB and naturalness:* besides possible right-handed neutrinos, the Higgs boson is the only Standard Model particle whose mass is not protected by a symmetry from the physics at energy scales much larger than M_W. To get a very rough estimate of what the contributions of New Physics to the Higgs mass could be, we assume that the effect of the new degrees of freedom can be approximated by computing Standard Model loop corrections to this mass, cutoff at a scale $\Lambda \gg M_W$ that is characteristic of the new phenomena. Then, the contributions to the Higgs mass at one loop are given by the diagrams in Fig. 1.1 with a cutoff Λ. They yield

$$\delta M_H^2 = \frac{3\Lambda^2}{16\pi^2 \langle \phi \rangle^2} (4m_t^2 - 2M_W^2 - M_Z^2 - M_H^2) \tag{1.15}$$

which is dominated by the top contribution for $M_H \ll 350\,\text{MeV}$. If, for naturalness reasons, we require that the physical squared Higgs mass is no less than a fraction f of the correction of Eq. (1.15), then we find that

$$\begin{aligned} \Lambda_{\text{nat}} &\le \frac{4\pi \langle \phi \rangle}{\sqrt{3f}} \frac{M_H}{\sqrt{4m_t^2 - 2M_W^2 - M_Z^2 - M_H^2}} \\ &\sim \frac{700\,\text{GeV}}{\sqrt{f}} \times \frac{(M_H/115\,\text{GeV})}{\sqrt{1 - \left(\frac{M_H - 115\,\text{GeV}}{310\,\text{GeV}}\right)^2}} \ . \end{aligned} \tag{1.16}$$
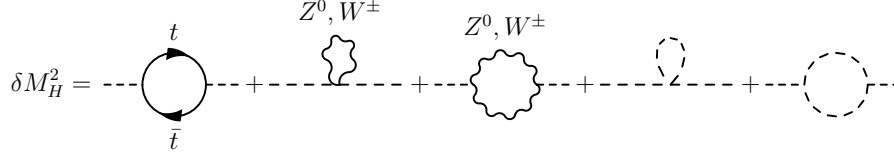
Fig. 1.1 Diagrams which contribute radiative corrections, δM_H^2, to the Higgs mass squared at one loop

Thus, if we allow at most 1% of fine tuning on the Higgs mass squared, Eq. (1.16) says that new physics must appear below $\Lambda_{\text{nat}} \sim 7\,\text{TeV}$.

2. *Gauge sector and flavor conserving $d = 6$ operators:* consider, for instance, $O_{WB} = g_1 g_2 (\phi^\dagger \sigma^a \phi) W_{\mu\nu}^a B_{\mu\nu}$, which couples the W bosons to the $U(1)_Y$ gauge boson B. Precision electroweak data, assuming that the Wilson coefficient of this operator is of order one, impose the following constraint on the scale of New Physics (Barbieri *et al.*, 2004):

$$\Lambda \gtrsim 5\,\text{TeV} \qquad 95\%\,\text{CL} . \tag{1.17}$$

3. *Flavor physics and, in particular, flavor changing neutral currents (FCNC):* consider, for instance, K^0-$\bar{K}^0$ mixing. In the absence of electroweak interactions, the long-lived K_L^0 is a CP odd state, whereas the short-lived K_S^0 is a CP even state. When these interactions are turned on, these two degenerate particles acquire a minuscule mass difference, which is measured experimentally to be:

$$\Delta M_K \equiv M_{K_L} - M_{K_S} \simeq 3.5 \times 10^{-12}\,\text{MeV} . \tag{1.18}$$

Consider now the contribution to ΔM_K of an arbitrary $d = 6$, $\Delta S = 2$ operator schematically written as $(\bar{d}s)(\bar{d}s)$:

$$\Delta M_K = 2 \times \frac{1}{2M_K} \frac{\text{Re}C_{\Delta S=2}^*}{\Lambda^2} \langle \bar{K}^0 | (\bar{s}d)(\bar{s}d) | K^0 \rangle . \tag{1.19}$$

Now, assuming that $\text{Re}C_{\Delta S=2}^* \sim 1$ and that the matrix element is of order the fourth power of a typical QCD scale, e.g. $\sim M_\rho^4$, we get

$$\Lambda > \frac{M_\rho^2}{\sqrt{M_K\,\Delta M_K}} \sim 10^3\,\text{TeV} \tag{1.20}$$

which is orders of magnitudes larger than the lower bound imposed by gauge sector and flavor conserving transitions, as well as than the upper bound imposed by naturalness.

Thus, if we do not make any assumptions about how the New Physics breaks flavor symmetries, we are forced to push this physics to very high scales. Said differently, flavor physics is sensitive to very high energy scales if the New Physics is allowed to have a flavor structure which differs from that of the Standard Model. Therefore, one assumption commonly made is that the New Physics breaks the flavor symmetries with the same Yukawa couplings as in the Standard Model. This assumption is called Minimal Flavor Violation (MFV). For instance, we might have, in the case of K^0-$\bar{K}^0$

mixing, the following operators contributing: $\frac{1}{\Lambda^2}(\bar{s}_R Y_{sd} d_L)^2$, $\frac{1}{\Lambda^2}(\bar{s}_L Y^*_{sd} Y_{sd} \gamma_\mu d_L)^2$, etc. I will leave you work out the corresponding scales, Λ, but they are certainly much lower and in line with those obtained from flavor-conserving physics.

1.2 Flavor physics phenomenology

As we shall see shortly in more detail, the Standard Model has a very rich and constrained flavor structure, which includes:

- mixing of quark flavors;
- CP violation by a unique invariant J (Jarlskog, 1985), discussed in Sec. 2.3.4;
- the absence of tree-level flavor changing neutral currents (FCNC).

All of these features are encapsulated in:

- the Cabibbo-Kobayashi-Maskawa (CKM) matrix (Cabibbo, 1963; Kobayashi and Maskawa, 1973)

$$V = \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} , \qquad (1.21)$$

  which is unitary. It has 3 mixing angles and a single phase, which is responsible for CP violation.
- the quark masses: m_q, with $q = u, d, s, c, b, t$.

For their discovery, in 1973, that Nature's CP violation and rich flavor structure can be well described when a third generation is added to the $SU(2)_L \times U(1)_Y$ electroweak model (Kobayashi and Maskawa, 1973), Kobayashi and Maskawa were awarded part of the 2008 Physics Nobel Prize.

Because this flavor structure is so intriguing and most probably contains important information about physics at much higher energies than currently explored, particle physicists have invested a considerable amount of effort in exploring it theoretically and experimentally over the past five decades. This exploration has multiple goals:

1) To determine from experiment the matrix elements of the CKM matrix V, which are important parameters of our fundamental theory.

2) To verify that the CKM description of quark flavor mixing and CP violation is correct, e.g.:

- Can all of the observed CP violation in the quark sector be explained in terms of a single phase?
- Is the measured matrix V unitary?

The latter can be tested by verifying whether

$$\sum_{D=d,s,b} |V_{UD}|^2 = 1 \qquad \text{and} \qquad \sum_{U=u,c,t} |V_{UD}|^2 = 1 . \qquad (1.22)$$

If either of these sums turn out to be less than 1, that would signal an additional generation or family. On the other hand, if either one is larger than 1, completely
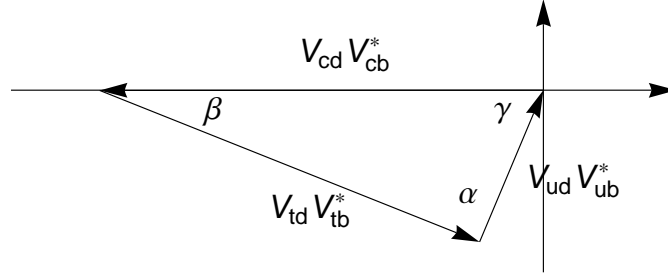
Fig. 1.2 The (db) unitarity triangle.

Fig. 1.3 From top to bottom, the (db), (sb) and (ds) unitary triangles, normalized by $V_{cD_1}V_{cD_2}^*/|V_{cD_1}V_{cD_2}^*|$ with $(D_1, D_2) = (d, b)$, (s, b) and (d, s) respectively, and drawn to a common scale.

new physics would have to be invoked. The unitarity of V also implies that the scalar product of any two distinct columns or rows of the matrix must vanish, i.e.

$$\sum_{U=u,c,t} V_{UD_1}V_{UD_2}^* = 0, \qquad \text{for } D_1 \neq D_2 , \tag{1.23}$$

$$\sum_{D=d,s,b} V_{U_1D}V_{U_2D}^* = 0, \qquad \text{for } U_1 \neq U_2 . \tag{1.24}$$

These relations can be represented as triangles in the complex plane, which are traditionally labeled by their unsummed flavors, i.e. (D_1, D_2) for those of Eq. (1.23) and (U_1, U_2) for those of Eq. (1.24). In the absence of CP violation, unitarity triangles would become degenerate. The (db) triangle is shown in Fig. 1.2. In Fig. 1.3, it is drawn to scale with two other triangles to give you a sense of the variety of unitarity triangles and the difficulties there may be in measuring some of their sides and angles.

The (db) triangle has been the focus of considerable experimental (LEP, B-factories, Tevatron, ...) and theoretical (QCD factorization, Soft Collinear Effective Theory (SCET), lattice QCD (LQCD), ...) effort in the last ten to fifteen years. With the arrival of the LHC and, in particular, the experiment LHCb, the focus is shifting from the study of the B_d towards the study of the B_s meson and thus toward investigations of the (sb) triangle. Here too, lattice QCD has a considerable role to play, most notably in the study of the B_s-$\bar{B}_s$ mass and width differences, of the leptonic decay $B_s \to \mu^+\mu^-$ or of the semileptonic decay $B_s \to \phi\mu^+\mu^-$.

The strategy here is to verify the unitarity of the CKM matrix by performing redundant measurements of:

- triangle sides with CP conserving decays,
- angles with CP violating processes,

and checking that the triangles indeed close.

3) To determine in what processes there is still room for significant New Physics contributions. For instance, $O(40\%)$ effects are still possible in B^0-$\bar{B}^0$ mixing from New Physics with a generic weak phase (Lenz *et al.*, 2010).

4) To constrain the flavor sectors of beyond the Standard Model (BSM) candidates. As we saw above, it is difficult to add new physics to the Standard Model without running into serious problems in the flavor sector.

5) To actually find evidence for beyond the Standard Model physics. This is most likely to be found in processes which are highly suppressed in the Standard Model, such as FCNC.

6) If new particles and interactions are discovered, it is important to investigate their quark and flavor structure.

All of these goals require being able to compute reliably and precisely flavor observables in the Standard Model or beyond. A high level of precision has been reached already on the magnitudes of individual CKM matrix elements (Charles *et al.*, 2005):

$$|V| = \begin{array}{c} \\ u \\ c \\ t \end{array} \begin{pmatrix} \overset{d}{0.97425^{+0.00018}_{-0.00018}} & \overset{s}{0.22543^{+0.00077}_{-0.00077}} & \overset{b}{0.00354^{+0.00016}_{-0.00014}} \\ 0.22529^{+0.00077}_{-0.00077} & 0.97342^{+0.00021}_{-0.00019} & 0.04128^{+0.00058}_{-0.00129} \\ 0.00858^{+0.00030}_{-0.00034} & 0.04054^{+0.00057}_{-0.00129} & 0.999141^{+0.000053}_{-0.000024} \end{pmatrix} , \tag{1.25}$$

assuming the correctness of the Standard Model and, in particular, CKM unitarity. The most poorly known CKM matrix elements are $|V_{ub}|$ and $|V_{td}|$, both with an uncertainty around 4%. Then come $|V_{ts}|$ and $|V_{cb}|$, with an uncertainty of about 2%. Thus, to have an impact in testing the CKM paradigm of quark flavor mixing and CP violation, and to take full advantage of LHCb results, the precision of theoretical predictions must be of order a few percent (better in many cases). This is no small challenge when nonperturbative QCD dynamics is involved.

1.3   Flavor physics and lattice QCD

Lattice QCD plays and will continue to play a very important role in flavor physics, by providing reliable calculations of nonperturbative strong interaction corrections to weak processes involving quarks.

The processes for which LQCD gives the most reliable predictions are those which involve a single hadron that is stable against strong interaction decay in the initial state and, at most, one stable hadron in the final state. Resonances (i.e. unstable hadrons) are much more difficult to contend with, especially if many decay channels are open. Similarly, final states with more than a single stable hadron are much more difficult, especially if these hadrons can rescatter inelastically. This will be discussed in much more detail in Sec. 3.7.

Thus, the processes typically considered for determining the absolute values of the CKM matrix elements are the following

$|V_{ud}|$ $\qquad\qquad$ $|V_{us}|$ $\qquad\qquad$ $|V_{ub}|$

$|V_{cd}|$ $\qquad\qquad$ $|V_{cs}|$ $\qquad\qquad$ $|V_{cb}|$

$|V_{ct}|$ $\qquad\qquad\qquad$ $|V_{ts}|$ $\qquad\qquad$ $|V_{tb}|$
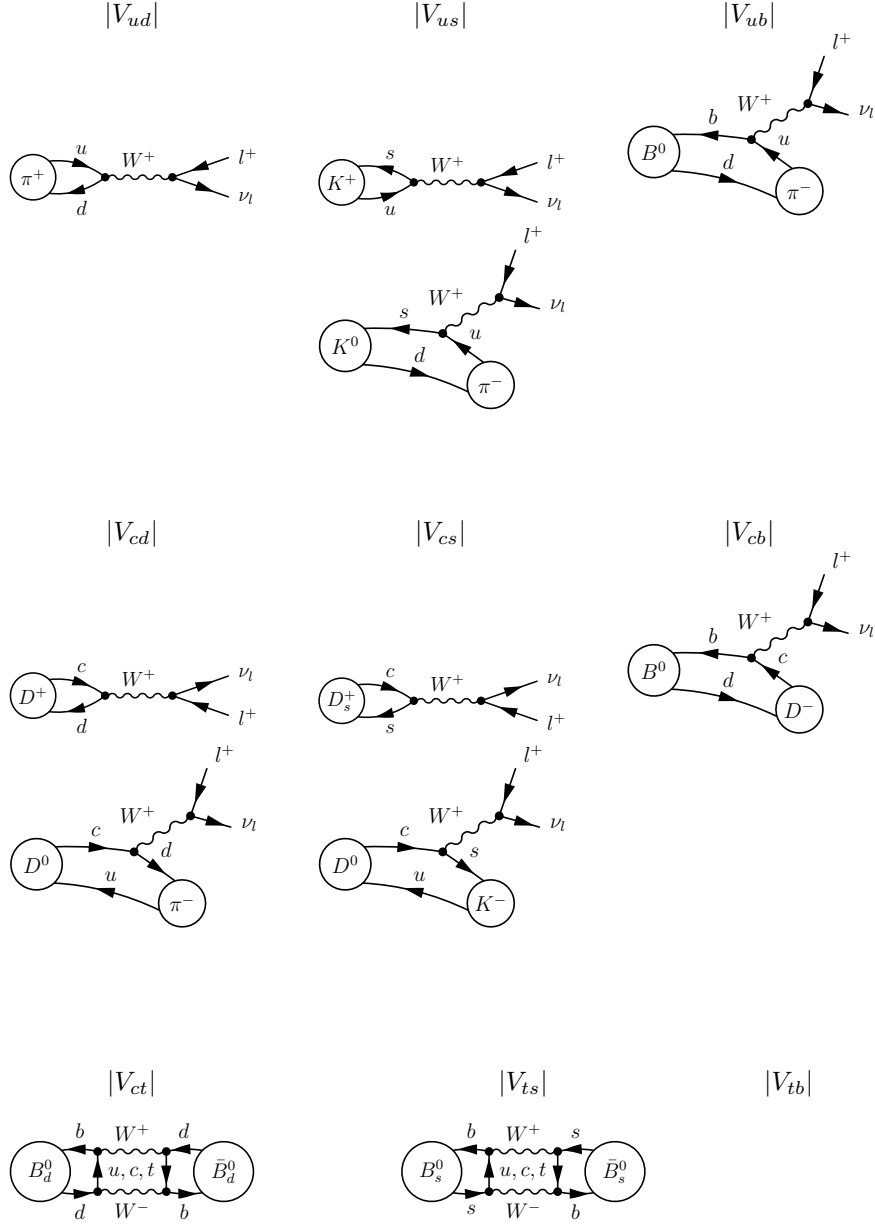
Now, to determine the unique CKM matrix phase or, more precisely, the CP violating parameter J, lattice QCD can have an important impact through the following processes:

- Indirect CP violation in $K \to \pi\pi$ decays. This occurs through the process of K^0-$\bar{K}^0$ mixing, which is given by the imaginary part

where the ellipsis stands for the other box contribution. It is a $|\Delta S| = 2$ FCNC that will be discussed in detail below.

- Direct CP violation in $K \to \pi\pi$ decays. The processes which contribute are given by the following $|\Delta S| = 1$ amplitudes

in the case of $K^0 \to \pi^+\pi^-$, where the ellipsis stands for missing diagrams similar to those drawn. The diagrams for $K^0 \to \pi^0\pi^0$ are analogous. Again, this particular phenomenon will be discussed in detail in the sequel.

1.4   Low-energy effective field theories of the Standard Model

With present knowledge and present computer resources, we cannot simulate the full Standard Model in lattice field theory calculations. In particular various degrees of freedom must be "eliminated" from the calculations for the following reasons:

- W, Z and t: there is no hope to be able to simulate these degrees of freedom whose masses are $M_{W,Z} \sim 80 \div 90\,\text{GeV}$ and $m_t \sim 175\,\text{GeV}$ on lattices which must be large enough to accommodate 135 MeV pions, i.e. with sizes $L \gtrsim 4/M_\pi \sim 6\,\text{fm}$. [4] Since we would also have to have $am_t \ll 1$, with a the lattice spacing, to guarantee

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[4]The factor of 4 in $4/M_\pi$ is a conservative rule-of-thumb estimate which guarantees that finite-volume corrections to stable hadron masses, proportional to $e^{-M_\pi L}$, are typically below the percent level.
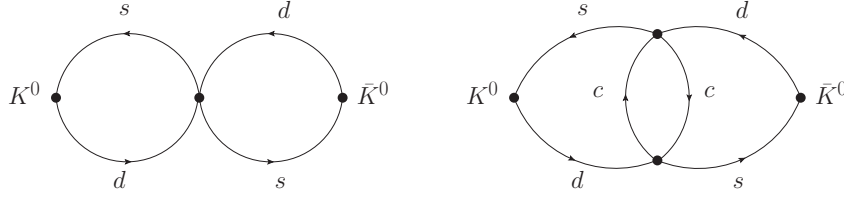
Fig. 1.4 Examples of correlation functions required for the lattice computation of the K^0-$\bar{K}^0$ mixing amplitude. The diagram on the left exhibits the type of three-point function with a four-quark operator insertion, required to obtain the K^0-$\bar{K}^0$ amplitude when the charm quark is integrated out. The diagram on the right shows a four-point function which is required when the charm quark is kept active.

controlled discretization errors, the number of points on the lattice would have to be $L/a \gg 4m_t/M_\pi \sim 5.2 \times 10^3$, which is beyond any foreseeable computing capabilities. Perhaps even more important, however, is the fact that we just do not know how to discretize nonabelian, chiral gauge theories (please see David's lecture notes in this volume (Kaplan, 2010)).

- b: even the b quark, with $m_b \sim 4.2\,\mathrm{GeV}$, would require lattices with $L/a \gg 120$, which is already too much for present technology.

- c: with $m_c \sim 1.3\,\mathrm{GeV}$, the charm is a borderline case, both on the lattice and in terms of QCD. On the lattice it can be included in simulations, but with $am_c \sim 0.35$ at best, discretization errors remain an important preoccupation. From the point of view of QCD, the charm is not quite a heavy quark–heavy quark effective theory is only marginally applicable since m_c is not much larger than typical QCD scales–and it is clearly not light–it is not in the regime of chiral perturbation theory. So its inclusion should be considered with care. In addition, its inclusion in weak processes can mean significantly more complicated correlation functions to compute. For instance, Fig. 1.4 illustrates the type of correlation functions required to determine the amplitude for K^0-$\bar{K}^0$ mixing, in the absence of charm (diagram on left) and in the presence of a dynamical charm quark (diagram on right). In the absence of charm, it is a rather standard three-point function which must be computed while in its presence, it is a four-point function, with two four-quark operator insertions. However, in certain circumstances, the inclusion of a dynamical charm quark significantly simplifies the renormalization of the weak effective theory, as briefly discussed in Sec. 3.8 for the $\Delta I = 1/2$ rule.

Fortunately, with the precisions required at present and in any foreseeable future, it is not necessary to include virtual W, Z, t and b contributions. The situation with the charm is less clear, as $(M_\rho/m_c)^2$ sea corrections can, in principle, play a role when percent precisions are reached. So in considering processes involving these massive particles, we can turn to effective field theories (EFTs) in which the W, Z, t, b and possibly c and τ are no longer dynamical degrees of freedom. Thus, we are left with an $SU(3)_c \times U(1)_{\mathrm{EM}}$ gauge theory of color and electromagnetism. This theory includes the virtual effects of the following degrees of freedom:

- 2 massless gauge bosons: the qluon, g, and the photon, γ
- 3 to 4 quarks: the u, d, s and possibly the c
- 2 to 3 leptons: the e, μ and possibly the τ
- 3 neutrinos: the ν_e, ν_μ and the ν_τ.

It also includes local operators of naive mass-dimension $d \geq 5$, which result from integrating out the heavy W, Z and t. Moreover, in this theory, the b–and possibly the c and the τ–are described by heavy fermion effective theories, in which the antiparticle of the fermion considered is integrated out. It is at this level that LQCD enters, to describe the nonperturbative effects of the strong interaction.

2

Standard Model and quark flavor mixing

As already discussed, the Standard Model has a highly constrained quark flavor structure, parametrized by the CKM matrix and the quark masses. We will now see more precisely how it arises and what its basic implications are.

2.1   On the origin of quark flavor mixing in the Standard Model

Let us look in more detail at the quark and gauge sectors of the Standard Model. With the notation (dim. rep. $SU(3)_c$, dim. rep. $SU(2)_L)_Y$, where "rep." stands for representation, the quark content of the Standard Model is given by

$$Q_L = \begin{pmatrix} U_L \\ D_L \end{pmatrix} \sim (3, 2)_{\frac{1}{2}}$$
$$U_R \sim (3, 1)_{2/3} \tag{2.1}$$
$$D_R \sim (3, 1)_{-1/3} \ ,$$

with $U = (u, c, t)^T$ and $D = (d, s, b)^T$. The coupling of these quarks with the gauge bosons is given by

$$\mathcal{L}_{g+q} = \cdots + \bar{Q}_L \slashed{D} Q_L + \bar{U}_R \slashed{D} U_R + D_R \slashed{D} D_R \ , \tag{2.2}$$

where the ellipsis stands for the gauge kinetic and self-interaction terms. This Lagrangian has the following global symmetries: $U(3)_L$ on Q_L, $U(3)_{U_R}$ on U_R and $U(3)_{D_R}$ on D_R.

Now let us look at the quark Yukawa terms. After spontaneous symmetry breaking by the Higgs field, keeping only the terms proportional to the Higgs v.e.v. $\langle \phi \rangle$, we have:

$$\mathcal{L}_m^q \xrightarrow{\langle \phi \rangle \neq 0} -\bar{U}_R M_U U_L - \bar{D}_R M_D D_L + \text{h.c.} \ , \tag{2.3}$$

where M_U and M_D are arbitrary 3×3 complex matrices. On these terms we perform the following set of flavor transformations which leave $\mathcal{L}_{g+q}$ invariant:

- the $SU(3)_{U_R}$ transformation: $U_R \to V_R^U U_R$,
- the $SU(3)_L$ transformation: $U_L \to V_L^U U_L$ and $D_L \to V_L^U D_L$,
- and the $SU(3)_{D_R}$ transformation: $D_R \to V_R^D D_R$,

with V_R^U, V_L^U and V_R^D such that:

$$M_U^d = V_R^{U\dagger} M_U V_L^U \ , \tag{2.4}$$

and

$$V_R^{D\dagger} M_D = M_D^d V_L^{D\dagger} \tag{2.5}$$

where $M_{U,D}^d$ are diagonal matrices with real positive entries which are the quark masses. The second equation defines a fourth unitary matrix V_L^D. Under these rotations, the quark mass Lagrangian transforms as

$$\mathcal{L}_m^q \to -\bar{U}_R M_U^d U_L - \bar{D}_R M_D^d [V_L^{D\dagger} V_L^U D_L] + \text{h.c.} \ . \tag{2.6}$$

The up quark mass matrix is diagonal in this basis, but not the down quark matrix. In addition, we have exhausted the flavor transformations allowed by $\mathcal{L}_{g+q}$. Thus, if we want to work in a mass basis (i.e. a basis in which all quark masses are diagonal), we have to perform the additional transformation:

- $D_L \to V_L^{U\dagger} V_L^D D_L$,

which is not a symmetry of $\mathcal{L}_{g+q}$. Clearly, the only terms in $\mathcal{L}_{g+q}$ which are affected are those which couple U_L and D_L. They are transformed in the following way:

$$
\begin{aligned}
\mathcal{L}_{CC}^q &= \frac{g_2}{\sqrt{2}} \bar{U}_L W\!\!\!\!/^{(+)} D_L + \text{h.c.} \\
&\to \frac{g_2}{\sqrt{2}} \bar{U}_L W\!\!\!\!/^{(+)} V D_L + \text{h.c.} \ ,
\end{aligned}
\tag{2.7}
$$

where CC stands for charged current and $V \equiv V_L^{U\dagger} V_L^D$ is the CKM matrix. All other terms are left unchanged. In particular, the neutral currents:

$$
\begin{aligned}
\mathcal{L}_{NC}^q &= \frac{g_2}{2} (\bar{U}_L, \bar{D}_L) W\!\!\!\!/^3 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} U_L \\ D_L \end{pmatrix} \\
&\quad + \frac{g_1}{6} (\bar{U}_L, \bar{D}_L) B\!\!\!/ \begin{pmatrix} U_L \\ D_L \end{pmatrix} \\
&\quad + \frac{2}{3} g_1 \bar{U}_R B\!\!\!/ U_R - \frac{1}{3} g_1 \bar{D}_R B\!\!\!/ D_R \ ,
\end{aligned}
\tag{2.8}
$$

which are flavor diagonal, remain diagonal in the mass basis. Moreover, the Higgs couples to fermions through their masses and therefore has a diagonal coupling to the quarks in the mass basis. The fact that all uncharged couplings remain diagonal in the mass basis implies that there are no tree level FCNC transitions in the Standard Model.

2.2   Properties of the CKM matrix

In this section, we look in more detail at what are the key properties of the CKM matrix.

2.2.1   Degrees of freedom of the CKM matrix

The flavor eigenstates, (d', s', b'), are related to the mass eigenstates, (d, s, b), through:

$$\begin{pmatrix} d' \\ s' \\ b' \end{pmatrix} = V \begin{pmatrix} d \\ s \\ b \end{pmatrix} \ , \tag{2.9}$$

where the CKM matrix is unitary, i.e. $V^\dagger V = V V^\dagger = 1$. Since V is a 3×3 complex matrix, it has 9 phases and 9 moduli. Unitarity imposes 3 real and 3 complex constraints. Thus, we are left with 6 phases and 3 moduli which, because of the normalization of the rows and columns to one, can be written as angles.

Now, aside from the CC interactions, all other terms involving quarks are diagonal in flavor, and have LL, LR, RL and RR chiral structures. Thus, we can perform vector (not axial) phase rotations on each flavor and leave all of these other terms invariant. However, under the phase rotations

$$U_{L,R} \to e^{i\theta_U} U_{L,R} \qquad \text{and} \qquad D_{L,R} \to e^{i\theta_D} D_{L,R} \ , \tag{2.10}$$

with $U = u$, c or t and $D = d$, s or b, the UD component of the CKM matrix transforms as

$$V_{UD} \to V_{UD}\, e^{i(\theta_D - \theta_U)} \ . \tag{2.11}$$

These transformations can be used to eliminate phases in V. Although there are 6 phases θ_U and θ_D, only 5 phase differences $\theta_D - \theta_U$ are independent. Thus, only 5 of the 6 phase can be eliminated.

We have now exhausted the field transformations that can be used to reduce the CKM matrix' degrees of freedom. Thus, V has 3 angles and 1 phase.

2.2.2   Standard parametrization of the CKM matrix

The idea behind this parametrization is to write V as a product of 3 rotations between pairs of generations, throwing the phase into the $1 \to 3$ rotation, so that it multiplies the smallest mixing coefficients. Thus,

$$V = R_{32}\, \mathrm{diag}\{1, 1, e^{i\delta}\} R_{31}\{1, 1, e^{-i\delta}\} R_{21} \ , \tag{2.12}$$

with the rotations

$$R_{21} = \begin{pmatrix} c_{12} & s_{12} & 0 \\ -s_{12} & c_{12} & 0 \\ 0 & 0 & 1 \end{pmatrix} \ , \tag{2.13}$$

$c_{12} = \cos\theta_{12}$ and $s_{12} = \sin\theta_{12}$, and similarly for the other rotations. This yields the following expression for the CKM matrix:

$$V = \begin{pmatrix} c_{12}c_{13} & c_{13}s_{12} & s_{13}e^{-i\delta} \\ -s_{12}c_{23} - c_{12}s_{23}s_{13}e^{i\delta} & c_{13}c_{23} - s_{12}s_{23}s_{13}e^{i\delta} & c_{13}s_{23} \\ s_{12}s_{23} - c_{12}c_{23}c_{13}e^{i\delta} & -c_{12}s_{23} - c_{23}s_{13}s_{13}e^{i\delta} & c_{13}c_{23} \end{pmatrix} \ , \tag{2.14}$$

and the angles are chosen to lie in the first quadrant. Note that this parametrization is not rephasing invariant.

2.2.3 Wolfenstein parametrization

Experimentally, it is found that $1 \gg s_{12} \gg s_{23} \gg s_{13}$, i.e. mixing gets smaller as one moves off the diagonal. It is convenient to exhibit this hierarchy by expanding V in powers of s_{12}, i.e. in the sine of the Cabibbo angle θ_{12} (Cabibbo, 1963; Gell-Mann and Levy, 1960). This yields the Wolfenstein parametrization (Wolfenstein, 1983). To implement this expansion, we define (Buras *et al.*, 1994)

$$\lambda \equiv s_{12} = \frac{|V_{us}|}{\sqrt{|V_{ud}|^2 + |V_{us}|^2}}$$

$$A\lambda^2 \equiv s_{23} = \frac{|V_{cb}|}{\sqrt{|V_{ud}|^2 + |V_{us}|^2}} \tag{2.15}$$

$$A\lambda^3(\rho + i\eta) \equiv s_{13}e^{i\delta} = V_{ub}^* .$$

and make the appropriate replacement in the standard parametrization of Eq. (2.14). Then,

$$V = \begin{pmatrix} 1 - \lambda^2/2 & \lambda & A\lambda^3(\rho - i\eta) \\ -\lambda & 1 - \lambda^2/2 & A\lambda^2 \\ A\lambda^3(1 - \rho - i\eta) & -A\lambda^2 & 1 \end{pmatrix} + O(\lambda^4) , \tag{2.16}$$

which clearly exhibits the hierarchy of mixing.

2.2.4 CP violation

Let us now see how CP violation arises in the Standard Model. Under parity, the charged W-boson fields transform as

$$W_\mu^{(\pm)}(x) \xrightarrow{P} W^{(\pm)\mu}(x_P) , \tag{2.17}$$

with $x_P = (x^0, -\vec{x})$. Similarly, under charge conjugation,

$$W_\mu^{(\pm)}(x) \xrightarrow{C} -W_\mu^{(\mp)}(x) . \tag{2.18}$$

Thus, under CP, these bosons transform as

$$W_\mu^{(\pm)}(x) \xrightarrow{CP} -W^{(\mp)\mu}(x_P) . \tag{2.19}$$

In my favorite Dirac spinor basis, the parity transform of a fermion field is given by:

$$\begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix}(x) \xrightarrow{P} \begin{pmatrix} \psi_R \\ \psi_L \end{pmatrix}(x_P) . \tag{2.20}$$

In this basis,

$$\gamma^\mu = \begin{pmatrix} 0 & \sigma^\mu \\ \bar{\sigma}^\mu & 0 \end{pmatrix} \qquad \text{and} \qquad \gamma^5 = \begin{pmatrix} -I & 0 \\ 0 & I \end{pmatrix} , \tag{2.21}$$

where I is the two-by-two unit matrix, $\sigma^\mu = (I, \vec{\sigma})$, $\bar{\sigma}^\mu = (I, -\vec{\sigma})$ and $\vec{\sigma}$ are the Pauli matrices. Clearly, parity is not a symmetry of the Standard Model since left and

right fermions belong to different representations of the Standard Model group. Under charge conjugation, we have

$$\psi(x) = \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix}(x) \xrightarrow{C} \psi^c(x) = \begin{pmatrix} i\sigma^2 \psi_R^* \\ -i\sigma^2 \psi_L^* \end{pmatrix}(x) = i\gamma^2\gamma^0\bar{\psi}^T(x) = C\bar{\psi}^T(x) \ . \quad (2.22)$$

Again, charge conjugation is clearly not a Standard Model symmetry. However, the CP operation,

$$\begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix}(x) \xrightarrow{CP} \begin{pmatrix} -i\sigma^2 \psi_L^* \\ i\sigma^2 \psi_R^* \end{pmatrix}(x_P) = \gamma^0 C\bar{\psi}^T(x_P) \ , \quad (2.23)$$

has a chance of being a symmetry transformation as it does not mix left and right-handed fields. Using the well known Pauli matrix identity, $\sigma^2\sigma^i\sigma^2 = -\sigma^{i*}$ and the anticommutation of fermion fields, the CC quark term of the Standard Model Lagrangian transforms, under CP, as:

$$\frac{g_2}{\sqrt{2}}\left\{\bar{U}_L \rlap{/}{W}^{(+)} V D_L + \bar{D}_L \rlap{/}{W}^{(-)} V^\dagger U_L\right\} \xrightarrow{CP} \frac{g_2}{\sqrt{2}}\left\{\bar{U}_L \rlap{/}{W}^{(+)} V^* D_L + \bar{D}_L \rlap{/}{W}^{(-)} V^T U_L\right\} \ . \tag{2.24}$$

Since $V^* \neq V$ in the presence of a nonvanishing phase, δ, CP is potentially violated in the Standard Model. We will see below what the necessary conditions for CP to be violated are.

2.3 CP violation and rephasing invariants

The standard parametrization of the CKM matrix V, given in Eq. (2.14), corresponds to a particular choice of quark field phases. Observables cannot depend on such choices. Therefore, it is important to find rephasing invariant combinations of CKM matrix elements.

2.3.1 Quadratic invariants

The moduli

$$I_{UD}^{(2)} \equiv |V_{UD}|^2 \ , \tag{2.25}$$

with $U = u, c, t$ and $D = d, s, b$, are clearly rephasing invariant. There are 9 of these.

Now, unitarity requires that:

$$\begin{cases} \sigma_U = \sum_{D=d,s,b} I_{UD}^{(2)} = 1 \\ \sigma_D = \sum_{U=u,c,t} I_{UD}^{(2)} = 1 \end{cases} , \tag{2.26}$$

which yields 6 constraints on the $I_{UD}^{(2)}$. However, we clearly have $\sum_U \sigma_U = \sum_D \sigma_D$, which means that there are only 5 independent constraints. In turn, this means that there are 4 independent quadratic invariants $I_{UD}^{(2)}$, which are obviously real.

2.3.2 Quartic invariants

We now define
$$I^{(4)}_{U_1 D_1 U_2 D_2} \equiv V_{U_1 D_1} V_{U_2 D_2} V^*_{U_1 D_2} V^*_{U_2 D_1} \ . \tag{2.27}$$
These products of CKM matrix elements are also clearly rephasing invariant, since for every field which one of the CKM factors in (2.27) multiplies, another factor multiplies its Dirac conjugate. In Eq. (2.27), U_1, U_2 (D_1, D_2) are chosen cyclically amongst u, c, t (d, s, b) so as to avoid $I^{(4)} = (I^{(2)})^2$ as well as to avoid obtaining complex conjugate invariants, e.g. $I^{(4)}_{U_1 D_2 U_2 D_1} = I^{(4)*}_{U_1 D_1 U_2 D_2}$. With these constraints, there are 9 invariants.

However, not all of these invariants are independent. Indeed, unitarity yields
$$\begin{cases} \sum_{D=d,s,b} V_{U_1 D} V^*_{U_2 D} = 0 & U_1 \neq U_2 \\ \sum_{U=u,c,t} V_{U D_1} V^*_{U D_2} = 0 & D_1 \neq D_2 \end{cases} . \tag{2.28}$$

This implies, in turn:
$$\begin{cases} V_{U_1 D_1} V^*_{U_2 D_1} = \sum_{D \neq D_1} V_{U_1 D} V^*_{U_2 D} & \text{(I)} \\ V_{U_1 D_1} V^*_{U_1 D_2} = \sum_{U \neq U_1} V_{U D_1} V^*_{U D_2} & \text{(II)} \end{cases} .$$

Multiplying both sides of (I) by $V_{U_2 D_2} V^*_{U_1 D_2}$ while maintaining the cyclicity of indices, yields
$$I^{(4)}_{U_1 D_1 U_2 D_2} = -|V_{U_1 D_1} V_{U_2 D_2}|^2 - I^{(4)}_{U_1 D_2 U_2 D_3} \qquad \text{(III)} \ .$$
Similarly, multiplying both sides of (II) by $V_{U_2 D_2} V^*_{U_2 D_1}$ gives
$$I^{(4)}_{U_1 D_1 U_2 D_2} = -|V_{U_2 D_1} V_{U_2 D_2}|^2 - I^{(4)}_{U_2 D_1 U_3 D_2} \qquad \text{(IV)} \ .$$

Thus, the 9 $I^{(4)}$'s can all be written in terms of $I^{(4)}_{udcs}$, for instance, and the 4 independent $I^{(2)}_{UD}$. Moreover, (III) and (IV) imply that all 9 $I^{(4)}$ have the same imaginary part.

2.3.3 Higher-order invariants

Higher-order invariants can, in fact, be written in terms of $I^{(2)}$s and $I^{(4)}$s. For instance, the sextic rephasing invariant $V_{U_1 D_1} V_{U_2 D_2} V_{U_3 D_3} V^*_{U_1 D_2} V^*_{U_2 D_3} V^*_{U_3 D_1}$ is equal to $I^{(4)}_{U_1 D_1 U_2 D_2} I^{(4)}_{U_2 D_1 U_3 D_3} / I^{(2)}_{U_2 D_1}$. This obviously fails in singular cases, but these will not be considered here because they are irrelevant in practice.

2.3.4 Jarlskog's invariant

This whole discussion of invariants implies that there is a unique, imaginary rephasing invariant combination of CKM matrix elements. This invariant must appear in all CP violating observables, because it is the imaginary component of the CKM matrix which is responsible for this violation. This invariant is known as the Jarlskog invariant (Jarlskog, 1985):
$$\begin{aligned} J \equiv \mathrm{Im}\, I^{(4)} &= c^2_{13} c_{12} c_{23} s_{12} s_{23} s_{13} s_\delta \\ &= \lambda^6 A^2 \bar\eta + O(\lambda^{10}) \ , \end{aligned} \tag{2.29}$$
where $\bar\eta = \eta(1 - \lambda^2/2)$. This, in turn, means that to have CP violation in the Standard Model, θ_{12}, θ_{23}, θ_{13} must not be 0 or $\pi/2$ and $\delta \neq 0, \pi$. Moreover, CP violation is

maximal for $s_\delta = 1$, $\theta_{12} = \theta_{23} = \pi/4$ and $s_{13} = 1/\sqrt{3}$. At that point, the Jarlskog invariant takes the value

$$J_{max} = \frac{1}{6\sqrt{3}} \simeq 0.1 \ . \tag{2.30}$$

However, global CKM fits yield (Charles *et al.*, 2005)

$$J = 2.96^{+18}_{-17} \times 10^{-5} \ll J_{max} \ , \tag{2.31}$$

i.e. CP violation in Nature is very far from being as large as it could be.

Instead of looking at the CKM matrix for a rephasing invariant measure of CP violation, we can go back to the mass matrices M_U and M_D. In Sec. 2.1, after performing only flavor transformations which are symmetries of $\mathcal{L}_{g+q}$, we reached the point where the quark mass term was given by Eq. (2.6)

$$\mathcal{L}^q_m \to -\bar{U}_R M^d_U U_L - \bar{D}_R M^d_D V^\dagger D_L + \text{h.c.} \ , \tag{2.32}$$

where V is the CKM matrix. Now, by performing the flavor symmetry transformation

$$D_R \longrightarrow V^\dagger D_R \ , \tag{2.33}$$

we obtain

$$\mathcal{L}^q_m \to -\bar{U}_R M^d_U U_L - \bar{D}_R V M^d_D V^\dagger D_L + \text{h.c.} \ . \tag{2.34}$$

In this equation, both M^d_U and $M^h_D \equiv V M^d_D V^\dagger$ are hermitian matrices. This means that the commutator $C_J \equiv [M^d_U, M^h_D]$ is pure imaginary. Since the only source of imaginary numbers in Eq. (2.34) is the phase of the CKM matrix, C_J carries information about CP violation in the Standard Model. However, C_J is not a rephasing invariant. Defining the matrices $P_U \equiv \text{diag}\{e^{-i\theta_u}, e^{-i\theta_c}, e^{-i\theta_t}\}$ and $P_D \equiv \text{diag}\{e^{-i\theta_d}, e^{-i\theta_s}, e^{-i\theta_b}\}$, under the rephasing operations of Eq. (2.10), C_J transforms as

$$C_J \to [M^d_U, P_D M^h_D P^\dagger_D] \ , \tag{2.35}$$

where P_U cancels against $P^\dagger_U$ in the first term, because M^d_U and P_U are diagonal. Nonetheless, $\det C_J$ is rephasing invariant, because M^d_U and P_D are diagonal. Thus, following Jarlskog (Jarlskog, 1985), we consider

$$\det C_J = 2iJ \times \prod_{U_1 > U_2} (m_{U_1} - m_{U_2}) \prod_{D_1 > D_2} (m_{D_1} - m_{D_2}) \ . \tag{2.36}$$

In light of what was discussed in the section on rephasing invariants, $\det C_J$ must be the only imaginary, rephasing-invariant quantity that can be obtained from the mass term of Eq. (2.34), which is the most general mass term that can be written for quarks in the Standard Model. This means that the presence of CP violation is the Standard Model is equivalent to $\det C_J \neq 0$. In turn this implies that there will be CP violation if and only if the conditions on the mixing angles and the phase of the CKM matrix given after Eq. (2.29) are obeyed, but also if and only if there are no mass degeneracies in the up and down quark sectors.

2.3.5 Unitarity triangle areas

As we saw earlier, the unitarity of the CKM matrix gives rise to 6 unitarity triangles, defined by Eqs. (1.23)–(1.24). The areas of the (D_1, D_2) triangles are given by

$$
\begin{aligned}
A_{D_1 D_2} &= \frac{1}{2} |V_{uD_1} V_{uD_2}^* \wedge V_{cD_1} V_{cD_2}^*| \\
&= \frac{1}{2} | - i\mathrm{Im}\, (V_{uD_1} V_{uD_2}^* V_{cD_1}^* V_{cD_2})| \\
&= \frac{1}{2} \mathrm{Im}\, I_{uD_1 cD_2}^{(4)} = \frac{1}{2} J \ ,
\end{aligned}
\tag{2.37}
$$

where the last line follows from Eq. (2.29). Similarly the areas of the (U_1, U_2) triangles are

$$
A_{U_1 U_2} = \frac{1}{2} \mathrm{Im}\, I_{U_1 dU_2 s}^{(4)} = \frac{1}{2} J \ .
$$

Thus, all 6 triangles have the same area, which is given by the Jarlskog invariant. Since CP violation can only arise if $J \neq 0$, none of the unitarity triangles can be degenerate if Standard Model CP violation is measured in Nature.

3
A lattice case study: $K \to \pi\pi$, CP violation and $\Delta I = 1/2$ rule

Having introduced the Standard Model and flavor physics, we now turn to an important set of processes that have been nagging theorists for over four decades: $K \to \pi\pi$ decays. These decays have been a rich source of information and of constraints on the weak interaction. In 1964 they provided the first evidence in Nature for indirect CP violation, which arises in the mixing of the neutral kaon with its antiparticle before the decay into two pion (Christenson *et al.*, 1964). Then, in 1999, CP violation which arises directly in the flavor-changing decay vertex was discovered in these same decays, after more than 20 years of experimental effort (Fanti *et al.*, 1999; Alavi-Harati *et al.*, 1999).

Currently these decays still give very important constraints on the CKM paradigm, through the measurement of indirect CP violation, parametrized by ϵ. And as far as we presently know, direct CP violation in these decays, parametrized by ϵ', may be harboring New Physics. Moreover, $K \to \pi\pi$ decays display what we believe are unusually large, and certainly poorly understood, nonperturbative QCD corrections, which go under the name of $\Delta I = 1/2$ rule.

At first sight the study of these decays is a perfect problem for the lattice. Only u, d and s (valence) quarks are involved, so that one expects controllable discretization errors. Of course, pions are light, which makes them difficult to simulate, and there are also two hadrons in the final state. But $SU(3)$ chiral perturbation theory (χPT) at LO relates $K \to \pi\pi$ to $K \to \pi$ and $K \to 0$ amplitudes which are simpler to compute (Bernard *et al.*, 1985). Moreover, χPT at NLO relates $K \to \pi\pi$ amplitudes obtained with heavier pions to the same amplitudes with physically light pions (Kambor *et al.*, 1990; Kambor *et al.*, 1991). Given the typical size of chiral corrections, one would expect that we could at least be able to get an $O(20 - 30\%)$ estimate of the relevant amplitudes. In addition to which we might expect good signals since only pseudoscalar mesons are involved.

Despite all of the positive indications that the lattice should be able to provide valuable information about these decays, all attempts to account for nonperturbative strong interaction effects have failed, except in the study of indirect CP violation. [1] And though much progress has been made on many aspects of these decays over the years, providing a fully quantitative description still remains an open problem. Thus,

---

[1] This was certainly true at the time of the school, but the situation has been moving quite fast since then [please see (Christ, 2010*a*; Liu, 2010; Sachrajda, 2010*a*) for an update].

I have chosen to focus on this particular topic in my discussion of the application of lattice methods to flavor phenomenology.

3.1 $K \to \pi\pi$ **phenomenology** [2]

Kaons have strong isospin 1/2, while pions have isospin 1. The weak decays of a kaon into two pions can thus occur through two channels in the isospin limit:

- the $\Delta I = 3/2$ channel, where the final two pions are in a state of isospin $I = 2$, a state which we label $(\pi\pi)_2$;
- the $\Delta I = 1/2$ channel, where the final two pions are in a state of isospin $I = 0$, a state which we label $(\pi\pi)_0$.

Decay into a two-pion state with isospin $I = 1$ is forbidden by Bose symmetry.

We denote the amplitudes for $K \to \pi\pi$ decays by:

$$T[K^0 \to (\pi\pi)_I] = iA_I e^{i\delta_I} \ , \tag{3.1}$$

where δ_I is the strong scattering phase of two pions in the isospin I, angular momentum $J = 0$ channel, defined through

$$T[(\pi\pi)_I \to (\pi\pi)_I] = 2e^{i\delta_I} \sin \delta_I \ . \tag{3.2}$$

In Eq. (3.1), K^0 is the flavor eigenstate with $I_3 = -1/2$ and strangeness $S = 1$: it is composed of a d and an $\bar{s}$ quark.

Using this notation, we have the following isospin decompositions for the $K \to \pi\pi$ amplitudes:

$$-iT[K^0 \to \pi^+\pi^-] = \frac{1}{\sqrt{6}}A_2 e^{i\delta_2} + \frac{1}{\sqrt{3}}A_0 e^{i\delta_0}$$

$$-iT[K^0 \to \pi^0\pi^0] = \sqrt{\frac{2}{3}}A_2 e^{i\delta_2} - \frac{1}{\sqrt{3}}A_0 e^{i\delta_0} \tag{3.3}$$

$$-iT[K^+ \to \pi^+\pi^0] = \frac{\sqrt{3}}{2}A_2 e^{i\delta_2} \ ,$$

where the coefficients of the various amplitudes are simply $SU(2)$ Clebsch-Gordan coefficients. If CP violation is present, then $A_I^* \neq A_I$.

Now, in the absence of CP violation, the two physical neutral kaon states K_S and K_L are also CP eigenstates: [3]

$$|K_{S/L}\rangle \simeq |K_\pm\rangle \equiv \frac{1}{\sqrt{2}}\left(|K^0\rangle \mp |\bar{K}^0\rangle\right) \ , \tag{3.4}$$

with $CP|K_\pm\rangle = \pm|K_\pm\rangle$. The CP even K_S decays only into two pions, while the CP odd K_L decays into three. Because of the phase space available to the decay products,

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[2]Here and in the following, we will assume that CPT is conserved. We will also work in the strong isospin symmetry limit.

[3]The CP transformation of the neutral kaon states is chosen here to be $CP|K^0(p)\rangle = -|\bar{K}^0(p_P)\rangle$ and $CP|\bar{K}^0(p)\rangle = -|K^0(p_P)\rangle$, where p_P is the parity transformed four-momentum $p = (p^0, -\vec{p})$. In the following, we will ignore the momentum labels unless they play a relevant role.

the former is much shorter lived than the latter, with a lifetime $\tau_S \sim 10^{-10}$ s versus $\tau_L \sim 5 \cdot 10^{-8}$ s. This explains the subscript S for short and L for long.

In Nature, the weak interaction breaks CP, and K_S and K_L are not pure CP eigenstates. As a result of K^0-$\bar{K}^0$ mixing through the weak interaction, we have

$$|K_{L/S}\rangle = \frac{1}{\sqrt{1+|\tilde{\epsilon}|^2}} \left(|K_{\mp}\rangle + \tilde{\epsilon}|K_{\pm}\rangle \right) \tag{3.5}$$

$$= \frac{1}{\sqrt{2}\sqrt{1+|\tilde{\epsilon}|^2}} \left((1+\tilde{\epsilon})|K^0\rangle \pm (1-\tilde{\epsilon})|\bar{K}^0\rangle \right) , \tag{3.6}$$

where $\tilde{\epsilon}$ is a small complex parameter.

The neutral kaons form a two state quantum mechanical system which can be described by a nonhermitian, 2-by-2 Hamiltonian:

$$H_{ij} = M_{ij} - \frac{i}{2}\Gamma_{ij} , \tag{3.7}$$

where $i, j = 1$ corresponds to K^0 and $i, j = 2$ to $\bar{K}^0$. CPT implies that $H_{11} = H_{22}$ and $H_{21} = H_{12}^*$. To determine the elements of this matrix, we first decompose the effective Hamiltonian for the Standard Model into a QCD+QED part, $H_{\mathrm{QCD+QED}}$, and a weak part, H_W, and work to second order in the weak interaction. Then,

$$H_{ij} = M_{K^0}\,\delta_{ij} + \frac{\langle i|H_W|j\rangle}{2M_{K^0}} + \frac{1}{2M_{K^0}} \sum_n\!\!\!\!\!\!\!\diagup \;\; \frac{\langle i|H_W|n\rangle\langle n|H_W|j\rangle}{M_{K^0} - E_n + i\epsilon} + \cdots , \tag{3.8}$$

where M_{K^0} is the mass common to K^0 and $\bar{K}^0$, as given in QCD and QED, and E_n is the energy of the intermediate state $|n\rangle$.

Now, Cauchy's theorem implies (with P the principal part)

$$\frac{1}{\omega - E + i\epsilon} = P\left(\frac{1}{\omega - E}\right) - i\pi\delta(E - \omega) , \tag{3.9}$$

where the first term on the RHS of this equation will yield the dispersive contribution to the Hamiltonian of Eq. (3.7) (i.e. the mass term) and the second term, the absorptive part (i.e. the width term). Then, the off-diagonal element of the mass matrix is

$$M_{12} = \frac{\langle K^0|H_{\Delta S=2}|\bar{K}^0\rangle}{2M_{K^0}} + \frac{1}{2M_{K^0}}P\sum_n\!\!\!\!\!\!\diagup \;\; \frac{\langle K^0|H_{\Delta S=1}|n\rangle\langle n|H_{\Delta S=1}|\bar{K}^0\rangle}{M_{K^0} - E_n} + \cdots , \tag{3.10}$$

where the term with the double insertion of the $\Delta S = 1$ Hamiltonian gives rise to long distance contributions, since the states $|n\rangle$ which can contribute are light. For instance, $|n\rangle$ can be a $\pi^+\pi^-$ state.

The off-diagonal element of the width matrix is given by the absorptive part of the integral:

$$\Gamma_{12} = \frac{1}{2M_{K^0}} \sum_n\!\!\!\!\!\!\diagup \;\; \langle K^0|H_{\Delta S=1}|n\rangle\langle n|H_{\Delta S=1}|\bar{K}^0\rangle(2\pi)\delta(E_n - M_{K^0}) \tag{3.11}$$

Now, the physical states K_L and K_S are the eigenstates of H_{ij} with eigenvalues $M_L - \frac{i}{2}\Gamma_L$ and $M_S - \frac{i}{2}\Gamma_S$, respectively. It is straightforward to express these quantities in terms of the M_{ij} and Γ_{ij}. Defining

$$\Delta M_K \equiv M_{K_L} - M_{K_S} \qquad \text{and} \qquad \Delta\Gamma_K \equiv \Gamma_{K_S} - \Gamma_{K_L} \ , \tag{3.12}$$

one obtains:

$$\frac{1 + \tilde{\epsilon}}{1 - \tilde{\epsilon}} = 2\frac{M_{12} - \frac{i}{2}\Gamma_{12}}{\Delta M_K + \frac{i}{2}\Delta\Gamma_K} \ . \tag{3.13}$$

Solving for $\tilde{\epsilon}$ gives us explicit expressions for computing the relationship of the physical eigenstates K_L and K_S to the flavor eigenstates K^0 and $\bar{K}^0$ through Eq. (3.6). It is worth noting that
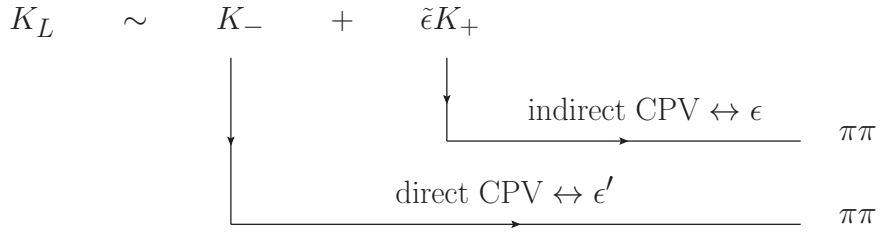
$$\Delta M_K \simeq 2M_{12} \qquad \text{and} \qquad \Delta\Gamma_K \simeq -2\Gamma_{12} \ , \tag{3.14}$$

to first nontrivial order in the weak phases.

Having implicitly worked out the relation between physical and flavor eigenstates, we return to $K \to \pi\pi$ decays. What is actually measured are the amplitude ratios

$$\eta_{00} \equiv \frac{T[K_L \to \pi^0\pi^0]}{T[K_S \to \pi^0\pi^0]} \qquad \text{and} \qquad \eta_{+-} \equiv \frac{T[K_L \to \pi^+\pi^-]}{T[K_S \to \pi^+\pi^-]} \ . \tag{3.15}$$

Experimentally, $|\eta_{00}| \simeq 2 \times 10^{-3}$, and $|\eta_{00}/\eta_{+-}| \simeq 1$ (Nakamura *et al.*, 2010). These ratios are clearly CP violating since K_L does not decay into two pions if CP is conserved. The CP violating decays $K_L \to \pi\pi$ can occur in two ways. As seen in Eq. (3.5), $|K_L\rangle$ can acquire a small CP even component proportional to $\tilde{\epsilon}|K_+\rangle$ through K^0-$\bar{K}^0$ mixing. This component can then decay into two pions without violating CP. However, the CP odd component of $|K_L\rangle$, proportional to $|K_-\rangle$, can directly decay into two pions if CP is violated in the decay. These two decay modes are illustrated in

$$K_L \qquad \sim \qquad K_- \qquad + \qquad \tilde{\epsilon}K_+$$

indirect CPV $\leftrightarrow \epsilon$

$\pi\pi$

direct CPV $\leftrightarrow \epsilon'$

$\pi\pi$

The first mode of decay is called indirect CP violation and is parametrized by a small number ϵ whose relation to $\tilde{\epsilon}$ will be given shortly. The second mode is call direct CP violation and is parametrized by an even smaller number ϵ'. These parameters are defined through

$$\epsilon = \frac{T[K_L \to (\pi\pi)_0]}{T[K_S \to (\pi\pi)_0]} \tag{3.16}$$

and

$$\epsilon' = \frac{1}{\sqrt{2}}\left(\frac{T[K_L \to (\pi\pi)_2]}{T[K_S \to (\pi\pi)_2]} - \epsilon\underbrace{\frac{T[K_S \to (\pi\pi)_2]}{T[K_S \to (\pi\pi)_0]}}_{\doteq\omega} \right) \ . \tag{3.17}$$

A little algebra allows us to relate these CP violating parameters to the measured quantities η_{00} and η_{+-}:

$$\eta_{00} = \epsilon - 2\frac{\epsilon'}{1 - \sqrt{2}\omega} \tag{3.18}$$

$$\eta_{+-} = \epsilon + \frac{\epsilon'}{1 + \omega/\sqrt{2}} \ . \tag{3.19}$$

Moreover, under the assumption that $(\pi\pi)_0$ dominates the sum for Γ_{12} in Eq. (3.11), the relationship of ϵ to $\tilde{\epsilon}$ can be calculated to be

$$\epsilon \simeq \frac{\tilde{\epsilon} + i\frac{\mathrm{Im}A_0}{\mathrm{Re}A_0}}{1 + i\tilde{\epsilon}\frac{\mathrm{Im}A_0}{\mathrm{Re}A_0}} \simeq \tilde{\epsilon} + i\frac{\mathrm{Im}A_0}{\mathrm{Re}A_0} \tag{3.20}$$

to first non-trivial order in the small CP violating quantities $\frac{\mathrm{Im}A_0}{\mathrm{Re}A_0}$ and $\tilde{\epsilon}$. A bit more algebra and some simplifications allow us to express ϵ, ϵ' and ω in terms of A_0, A_2 and $\mathrm{Im}M_{12}$ (de Rafael, 1995) which, in principle, can be calculated using lattice QCD:

$$\omega \simeq \frac{\mathrm{Re}A_2}{\mathrm{Re}A_0}e^{i(\delta_2 - \delta_0)} \tag{3.21}$$

$$\epsilon \simeq e^{i\phi_\epsilon} \sin\phi_\epsilon \left\{ \frac{\mathrm{Im}M_{12}}{\Delta M_K} + \frac{\mathrm{Im}A_0}{\mathrm{Re}A_0} \right\} \tag{3.22}$$

$$\epsilon' \simeq \frac{e^{i(\delta_2 - \delta_0)}}{\sqrt{2}}\mathrm{Im}\frac{A_2}{A_0} \ , \tag{3.23}$$

where the phase of ϵ is approximately given by $\phi_\epsilon \simeq (2\phi_{+-} + \phi_{00})/3 \sim \pi/4$, with ϕ_{+-} and ϕ_{00} the phases of η_{+-} and η_{00}, respectively. [4] In the expression for ϵ', the imaginary part of A_2/A_0 measures the relative reality of A_2 and A_0, which is what we need for direct CP violation since the latter must arise from the interference between the two available decay channels. Note that with the approximations used here, Eq. (3.14) gave $\Delta M_K \simeq 2\mathrm{Re}M_{12}$, where $\mathrm{Re}M_{12}$ also could, in principle, be computed on the lattice.

Experimentally, the various quantities which describe the K^0-$\bar{K}^0$ system and $K \to \pi\pi$ decays are well measured (Nakamura *et al.*, 2010):

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[4]In many phenomenological studies, ϕ_ϵ is fixed to $\pi/4$ and $\frac{\mathrm{Im}A_0}{\mathrm{Re}A_0}$ is neglected. However, at the levels of accuracy currently reached in the computation of the local contributions to $\mathrm{Im}M_{12}$, these approximations are becoming too crude. This has been emphasized in (Buras and Guadagnoli, 2008), where the implications of an estimate of $\frac{\mathrm{Im}A_0}{\mathrm{Re}A_0}$ and of the deviation of ϕ_ϵ from $\pi/4$ has been investigated. Moreover, as explained in (Buras *et al.*, 2010), if $\frac{\mathrm{Im}A_0}{\mathrm{Re}A_0}$, which approximates $-\frac{\mathrm{Im}\Gamma_{12}}{2\mathrm{Re}\Gamma_{12}}$, is included in Eq. (3.22), consistency requires that one also account for long distance contributions to $\mathrm{Im}M_{12}$.

$$\Delta M_K = (3.483 \pm 0.006) \times 10^{-12}\,\mathrm{MeV} \qquad [0.2\%] \tag{3.24}$$

$$\frac{1}{|\omega|} \simeq \left| \frac{A_0}{A_2} \right| \simeq 22.4 \qquad (\Delta I = 1/2 \text{ rule}) \tag{3.25}$$

$$|\epsilon| \simeq (2|\eta_{+-}| + |\eta_{00}|)/3 = (2.228 \pm 0.011) \times 10^{-3} \qquad [0.5\%] \tag{3.26}$$

$$\phi_\epsilon \simeq (2\phi_{+-} + \phi_{00})/3 = 43.51 \pm 0.05 \qquad [0.1\%] \tag{3.27}$$

$$\mathrm{Re}\frac{\epsilon'}{\epsilon} \simeq \left(1 - \left| \frac{\eta_{00}}{\eta_{+-}} \right| \right) = (1.65 \pm 0.26) \times 10^{-3} \qquad [16\%] \ . \tag{3.28}$$

Using lattice QCD, the weak matrix element relevant for the short-distance, Standard Model contribution of $|\epsilon|$ has been calculated with a precision of less than 3% (see (Lellouch, 2009; Lubicz, 2009; Sachrajda, 2010a; Colangelo *et al.*, 2010) for recent reviews). We are just beginning to provide phenomenologically relevant information for the $\Delta I = 1/2$ rule $|A_0/A_2|$ (Sachrajda, 2010a; Liu, 2010; Christ, 2010a), but $\mathrm{Re}(\epsilon'/\epsilon)$ is still out of reach for the moment (Sachrajda, 2010a). Moreover, as already mentioned and discussed further below, ΔM_K has long distance contributions which make its determination on the lattice difficult. However, for that also, progress has been made (Christ, 2010b).

3.2 K^0-$\bar{K}^0$ mixing in the Standard Model

As we have just seen, $\bar{K}^0$-K^0 mixing arises from the $\Delta S = 2$, $s\bar{d} \to \bar{s}d$ FCNC. This mixing is responsible for the K_L-K_S mass difference, ΔM_K, and indirect CP violation in $K \to \pi\pi$ decays.

In the Standard Model, it occurs at one loop through diagrams such as (Glashow, Iliopoulos and Maiani, 1970; Gaillard and Lee, 1974b)

$$\tag{3.29}$$
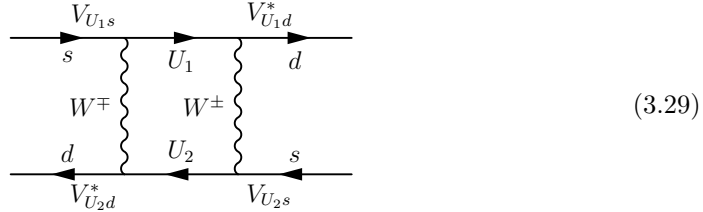
Setting the external four-momenta to zero, the amplitude associated with this diagram is

$$-i\mathcal{M} = \left(\frac{-ig_2}{\sqrt{2}} \right)^4 \int \frac{d^4 k}{(2\pi)^4} i D_{\mu\nu}^W(k) i D_{\rho\sigma}^W(k) \left(\bar{v}_{dL} \gamma_\mu i S(k) \gamma_\sigma v_{sL} \right) \left(\bar{u}_{dL} \gamma_\nu i S(k) \gamma_\rho u_{sL} \right) \ , \tag{3.30}$$

where the u's and v's are the usual particle and antiparticle spinor wavefunctions, and we have defined the amplitude with a minus sign for convenience. The W boson propagator in Feynman gauge is

$$D_{\mu\nu}^W(k) = \frac{-g_{\mu\nu}}{k^2 - M_W^2 + i\epsilon} \tag{3.31}$$

and the sum of the up quark propagators,

$$S(k) = \sum_{U=u,c,t} \frac{\lambda_U}{\not{k} - m_U + i\epsilon} \ , \tag{3.32}$$

with $\lambda_U \equiv V_{Us}V_{Ud}^*$.

The unitarity of the CKM matrix implies that $\sum_{U=u,c,t} \lambda_U = 0$. Thus, we have (dropping $i\epsilon$ for the moment)

$$S(k) = \sum_{U=c,t} \lambda_U \left(\frac{1}{\not{k} - m_U} - \frac{1}{\not{k} - m_u} \right) \ . \tag{3.33}$$

From this we see the GIM mechanism (Glashow *et al.*, 1970) in action: if $m_u = m_c = m_t$ there would be no K^0-$\bar{K}^0$ mixing. In fact, this process was used to estimate the charm quark mass before it was actually discovered (Gaillard and Lee, 1974b).

After performing some Dirac algebra, we find:

$$\mathcal{M} = \frac{G_F^2 M_W^2}{2\pi^2} (\lambda_t^2 T_{tt} + \lambda_c^2 T_{cc} + 2\lambda_c \lambda_t T_{ct}) \times (\bar{v}_{dL}\gamma_\mu v_{sL})(\bar{u}_{dL}\gamma^\mu u_{sL}) \ , \tag{3.34}$$

where we have used $G_F = g_2^2/(4\sqrt{2}M_W^2)$. Setting $m_u = 0$,

$$T_{U_1 U_2} = \frac{4i}{\pi^2 M_W^2} \int d^4k \frac{1}{k^2(1 - k^2/M_W^2)^2} \frac{m_{U_1}^2}{k^2 - m_{U_1}^2} \frac{m_{U_2}^2}{k^2 - m_{U_2}^2} \ . \tag{3.35}$$

With the spinor wavefunction factors appropriately replaced by quark field operators, $\mathcal{M}$ can be interpreted as an effective Hamiltonian whose matrix element between a K^0 and a $\bar{K}^0$ state yields the off diagonal matrix element (3.10) of the mass matrix of Eq. (3.7). Of course, to obtain the full effective $\Delta S = 2$ Hamiltonian, one must include the contributions of all of the diagrams which contribute to the process (Inami and Lim, 1981). [5]

Now, the values of the CKM matrix elements as well as of the masses m_u, m_c and m_t imply that $\mathrm{Re}M_{12} \gg \mathrm{Im}M_{12}$ and that $\mathrm{Re}M_{12}$ is dominated by the cc term. Naively,

$$\frac{G_F^2 M_W^2}{4\pi^2} T_{cc} = \frac{iG_F^2}{\pi^4} \int d^4k \frac{m_c^4}{(k^2 + i\epsilon)[k^2 - m_c^2 + i\epsilon]^2} + O\left(\frac{1}{M_W^6}\right)$$
$$= \frac{G_F^2 m_c^2}{\pi^2} + O\left(\frac{1}{M_W^6}\right) \ . \tag{3.36}$$

However, a closer look at this loop integral indicates that it is dominated by momenta in the range between 0 and m_c and we should not forget that all sorts of gluons with

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[5]Eq. (3.34) and the amplitudes associated with the other contributing diagrams must be multiplied by 1/2 if their spinors factors are replaced by operators to yield the effective $\Delta S = 2$ Hamiltonian. Indeed, the operator $(\bar{d}_L\gamma_\mu s_L)(\bar{d}_L\gamma^\mu s_L)$ has twice as many contractions with the four external quark states as there really are. These extra contractions correspond to a doubling of the individual box diagrams.

or without quark loops can be exchanged between the quarks in the diagram. Since these momenta include scales of $O(\Lambda_{\mathrm{QCD}})$ or below, it is clear that α_s corrections are out of control and $\mathrm{Re}M_{12}$ cannot be calculated in this way.

Said differently, box diagrams, such as the one of Eq. (3.29), cannot be viewed like a point interaction, but rather receive long-distance contributions from intermediate $c\bar{c}$ states. In the language of Eq. (3.10), these diagrams contribute to the second term through $(\bar{d}_L\gamma_\mu s_L)(\bar{c}_L\gamma_\mu c_L)$ effective operators in $\mathcal{H}_{\Delta S=1}$.

The situation is very different for the calculation of the CP violating parameter $\epsilon \sim \mathrm{Im}M_{12}/\mathrm{Re}M_{12}$ [6]. Indeed, indirect CP violation in $K \to \pi\pi$ decays comes from the interference between the following types of contributions
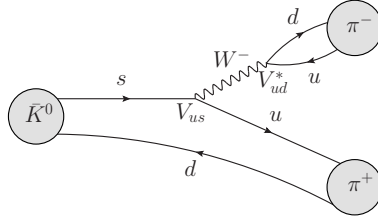
and
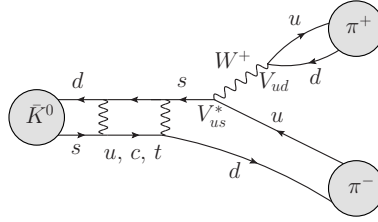
So, the relative weak phase between the two types of contributions is $\arg\{(\lambda_u^*)^2 M_{12}\}$ and thus, what we really have is

$$\epsilon \sim \frac{\mathrm{Im}\left[(\lambda_u^*)^2 M_{12}\right]}{\mathrm{Re}\left[(\lambda_u^*)^2 M_{12}\right]} \ , \tag{3.37}$$

where the $(\lambda_u^*)^2$ had been canceled in earlier expressions, using the fact that λ_u is real in our conventions.

Now, using Eq. (3.34) with the replacement of wavefunctions by operators discussed after Eq. (3.35), we have:

$$(\lambda_u^*)^2 M_{12} \sim \frac{G_F^2 M_W^2}{16\pi^2}\Big(\underbrace{(\lambda_u^*\lambda_t)^2}_{I_{udts}^{(4)}} T_{tt} + \underbrace{(\lambda_u^*\lambda_c)^2}_{I_{udcs}^{(4)}} T_{cc} + 2(\lambda_u^*\lambda_c)(\lambda_u^*\lambda_t)T_{ct}\Big)$$
$$\times \langle K^0|(\bar{d}s)_{V-A}(\bar{d}s)_{V-A}|\bar{K}^0\rangle \ , \tag{3.38}$$

where

[6]For the sake of clarity, we neglect here the small contribution to ϵ from $\frac{\mathrm{Im}A_0}{\mathrm{Re}A_0}$ (see Eq. (3.22)).

$$(\bar{d}s)_{V-A} = \bar{d}\gamma_\mu(1-\gamma_5)s \qquad (3.39)$$

and where the $I^{(4)}$ are the quartic rephasing invariants defined in Eq. (2.27). As shown in Sec. 2.3.2, $\mathrm{Im}I^{(4)}_{udcs} = J = -\mathrm{Im}I^{(4)}_{udts}$, where J is the Jarlskog invariant. Therefore,

$$\mathrm{Im}[(\lambda_u^*)^2 M_{12}] \sim \frac{g_2^4}{8M_W^4} J \left\{ \mathrm{Re}(\lambda_u^*\lambda_t)(T_{tt} - T_{ct}) - \mathrm{Re}(\lambda_u^*\lambda_c)(T_{cc} - T_{ct}) \right\}$$
$$\times \langle K^0 | (\bar{d}s)_{V-A}(\bar{d}s)_{V-A} | \bar{K}^0 \rangle , \qquad (3.40)$$

and J appears as it should in a CP violating quantity.

Moreover, the integrals in $(T_{tt} - T_{ct})$ and $(T_{cc} - T_{ct})$ are dominated by momenta between m_c and m_t. The same is true of the integrals which appear in the other diagrams (Inami and Lim, 1981) that contribute to this $\Delta S = 2$ process. That means that the QCD corrections are calculable to the extent that m_c can be considered a perturbative scale. Thus, under this assumption, and using the experimental value of ΔM_K in lieu of $\mathrm{Re}\left[(\lambda_u^*)^2 M_{12}\right]$, we can reliably calculate ϵ with the replacement

i.e. by replacing the box diagram with the local, four-quark operator of Eq. (3.40), and the appropriate short-distance QCD corrections, omitted here. As mentioned in footnote 4, corrections to this approximation have been examined in (Buras *et al.*, 2010).

3.3   The theory of K^0-$\bar{K}^0$ mixing

The calculation of M_{12} of the previous section has actually been performed to leading-log (LL) (Vainshtein *et al.*, 1977b; Witten, 1977; Vainshtein *et al.*, 1977a; Gilman and Wise, 1983) and next-to-leading-log order (NLL) (Buras *et al.*, 1990) in QCD (for a review see (Buchalla *et al.*, 1996)). The resulting NLL, $\Delta S = 2$ effective Hamiltonian is given by

$$\mathcal{H}_{\Delta S=2} = \frac{G_F^2}{16\pi^2} M_W^2 \left[\lambda_t^2 \eta_{tt} S_{tt} + \lambda_c^2 \eta_{cc} S_{cc} + 2\lambda_c\lambda_t\eta_{ct} S_{ct} \right]$$
$$\times C(\mu) \times (\bar{d}s)_{V-A}(\bar{d}s)_{V-A} , \qquad (3.41)$$

where the running of matrix elements of the four quark operator is canceled by the coefficient $C(\mu)$, the $S_{qq'}$ are the Inami-Lim functions (Inami and Lim, 1981) which

correspond to the electroweak box contributions in the absence of the strong interaction, and the $\eta_{qq'}$ are short-distance QCD corrections. In Eq. (3.41) all Standard Model degrees of freedom with masses down to, and including, that of the charm quark are integrated out. Thus, in Eq. (3.41), all QCD quantities must be evaluated with *three* active quark flavors.

It is useful to consider the case of a general number of active quark flavors, N_f, and of colors, N_c, when discussing the running of this $\Delta S = 2$ operator. Indeed, the running is the same for other Standard Model, $\Delta F = 2$ operators, such as $\Delta B = 2$ and $\Delta C = 2$, except that N_f must be chosen appropriately. Moreover, working with general N_c allows one to consider the large-N_c limit, to be discussed shortly. With $a_s \equiv \alpha_s/4\pi$, the running of α_s and of $C(\mu)$ is given by:

$$\frac{d\ln a_s}{d\ln \mu^2} = -\beta(a_s) = -\beta_0 a_s - \beta_1 a_s^2 + O(a_s^3) \, , \tag{3.42}$$

$$\frac{d\ln C}{d\ln \mu^2} = \gamma(a_s) = \gamma_0 a_s + \gamma_1 a_s^2 + O(a_s^3) \, , \tag{3.43}$$

where $\beta(a_s)$ is the QCD β function and $\gamma(a_s)$ is the anomalous dimension of the $\Delta S = 2$ operator. It is well known that β_0, β_1, and that LO anomalous dimensions are renormalization scheme independent. At two loops, we have (Nakamura *et al.*, 2010)

$$\beta_0 = \frac{11N_c - 2N_f}{3} \, , \qquad \beta_1 = \frac{34}{3}N_c^2 - \frac{10}{3}N_c N_f - 2C_F N_f \, , \qquad C_F = \frac{N_c^2 - 1}{2N_c} \, . \tag{3.44}$$

and, in the $\overline{\text{MS}}$-NDR scheme for γ_1,

$$\gamma_0 = 3\frac{N_c - 1}{N_c} \, , \qquad \gamma_1 = \frac{N_c - 1}{4N_c}\left[-21 + \frac{57}{N_c} - \frac{19}{3}N_c + \frac{4}{3}N_f\right] \, . \tag{3.45}$$

It is straightforward to integrate Eq. (3.42):

$$\frac{1}{a_s(\mu)} - \beta_0 \ln\left(\frac{\mu}{\mu_0}\right)^2 + \frac{\beta_1}{\beta_0} \ln\left[\frac{a_s(\mu)}{1 + (\beta_1/\beta_0)a_s(\mu)}\right] \tag{3.46}$$

$$= \frac{1}{a_s(\mu_0)} + \frac{\beta_1}{\beta_0} \ln\left[\frac{a_s(\mu_0)}{1 + (\beta_1/\beta_0)a_s(\mu_0)}\right]$$

For reasonably small $a_s(\mu_0) \ln(\mu/\mu_0)^2$, the coupling at μ can be related to the one at μ_0 through:

$$a_s(\mu) = a_s(\mu_0) \left\{1 - \beta_0 a_s(\mu_0) \ln\left(\frac{\mu}{\mu_0}\right)^2 - a_s(\mu_0)^2 \ln\left(\frac{\mu}{\mu_0}\right)^2 \right. \tag{3.47}$$

$$\left. \times \left[\beta_1 - \beta_0^2 \ln\left(\frac{\mu}{\mu_0}\right)^2\right]\right\} + O(a_s^3) \, . \tag{3.48}$$

Alternatively, we can define Λ_{QCD} as the value of μ_0 at which $a_s(\mu_0)$ is infinite, yielding:

$$a_s(\mu) = \frac{1}{\beta_0 \ln \frac{\mu^2}{\Lambda_{\rm QCD}^2}} \left[1 + \frac{\beta_1 \ln \ln \frac{\mu^2}{\Lambda_{\rm QCD}^2}}{\beta_0^2 \ln \frac{\mu^2}{\Lambda_{\rm QCD}^2}} + \cdots \right] \ . \tag{3.49}$$

It is also straightforward to integrate Eq. (3.43),

$$\frac{C(\mu)}{C(\mu_0)} = \exp\left\{ -\int_{a_s(\mu_0)}^{a_s(\mu)} \frac{da_s}{a_s} \frac{\gamma(a_s)}{\beta(a_s)} \right\} \ . \tag{3.50}$$

The coefficient $C(\mu)$ is only defined up to an integration constant. For consistency with Eq. (3.41), I consider

$$C(\mu) = [4\pi a_s(\mu)]^{-\gamma_0/\beta_0} \exp\left\{ -\int_0^{a_s(\mu)} \frac{da_s}{a_s} \left[\frac{\gamma(a_s)}{\beta(a_s)} - \frac{\gamma_0}{\beta_0} \right] \right\} \ . \tag{3.51}$$

Thus, at NLO

$$C(\mu) = [4\pi a_s(\mu)]^{-\gamma_0/\beta_0} \left[1 + \frac{\beta_1}{\beta_0} a_s + O(a_s^2) \right]^{\left(\frac{\gamma_0}{\beta_0} - \frac{\gamma_1}{\beta_1} \right)} \ . \tag{3.52}$$

For the Standard Model $\Delta F = 2$ operator relevant for K^0-$\bar{K}^0$ mixing, we use the anomalous dimension coefficients of Eq. (3.45), with $N_f = 3$ and, of course, $N_c = 3$. Thus, at NLO,

$$C(\mu) = \alpha_s(\mu)^{-2/9} \left[1 + \frac{307}{162} \frac{\alpha_s(\mu)}{4\pi} \right] \ . \tag{3.53}$$

Then, in Eq. (3.41) the QCD corrections $\eta_{qq'}$ are of the form

$$\eta_{qq'} \propto \frac{[1 + O(\alpha_s)]}{C(m_c)} \ , \tag{3.54}$$

and where $x_q \equiv (m_q/M_W)^2$. For details, please see (Buchalla *et al.*, 1996).

To calculate ϵ, we must compute the matrix element $\langle K^0|(\bar{d}s)_{V-A}(\bar{d}s)_{V-A}(\mu)|\bar{K}^0\rangle$, where the kaons are at rest. This is clearly a nonperturbative QCD quantity because the typical energies of the quarks within the kaons are on the order of $100\,{\rm MeV}$, a regime where perturbation theory fails and confinement effects must be taken into account. This is where lattice QCD enters. [7]

For historical reasons, and because it is very convenient in lattice computations, we define a normalized matrix element

$$B_K(\mu) \equiv \frac{\langle \bar{K}^0|(\bar{s}d)_{V-A}(\bar{s}d)_{V-A}(\mu)|K^0\rangle}{\frac{8}{3}\langle \bar{K}^0|\bar{s}\gamma_\mu\gamma_5 d|0\rangle\langle 0|\bar{s}\gamma_\mu\gamma_5 d|K^0\rangle} \ , \tag{3.55}$$

where we have considered the $\Delta S = -2$ matrix element to conform with convention. The benefit of this normalization on the lattice, is that the resulting B_K parameter

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[7]Here again we choose to neglect the small contribution to ϵ from $\frac{{\rm Im}A_0}{{\rm Re}A_0}$. Computing it on the lattice is a whole other project which is related to the computation of ϵ'. That computation goes beyond the presentation I wish to make here.

is dimensionless. Therefore it does not suffer from ambiguities due to scale setting, something which was particularly bad in old quenched-calculation days. Moreover, the numerator and denominator are very similar, and both statistical and systematic uncertainties cancel in the ratio. Of course, the convenience of this normalization would be limited if the denominator were an unknown, nonperturbative quantity. However, the matrix elements in the denominator define the leptonic decay constant of the kaon, f_K, [8]

$$\langle 0|\bar{s}\gamma_\mu\gamma_5 d(x)|K^0(p)\rangle = if_K p_\mu e^{-ip\cdot x} , \qquad (3.56)$$

which is well measured experimentally or straightforward to compute on the lattice. (In the convention used here, $f_K \simeq 156\,\mathrm{MeV}$.) Thus, once the B-parameter has been computed, the normalizing factor is a known quantity and the desired matrix element is easily obtained, from

$$\langle \bar{K}^0| \underbrace{(\bar{s}d)_{V-A}(\bar{s}d)_{V-A}(\mu)}_{O^{\mathrm{SM}}_{\Delta S=-2}} |K^0\rangle = \frac{8}{3} f_K^2 M_K^2 B_K(\mu) , \qquad (3.57)$$

where M_K^2 is best taken from experiment.

Historically, the denominator in Eq. (3.55) was an approximation used to estimate the matrix element of $O^{\mathrm{SM}}_{\Delta S=-2}$. It is called the vacuum saturation approximation, or VSA for short. It is obtained by inserting the vacuum in all possible ways between all possible quark-antiquark field pairs formed from the fields of the four-quark operators, using Fierz transformations if necessary to bring the fields together. For the case of interest here,

$$\langle 0|\bar{s}_b\gamma_\mu(1-\gamma_5)d^a(x)|K^0(p)\rangle = -i\frac{\delta_b^a}{N_c} f_K p_\mu e^{-ip\cdot x} , \qquad (3.58)$$

where a and b are color indices and the dependence on the number of colors $N_c = 3$ is made explicit. Therefore

$$\langle \bar{K}^0|O^{\mathrm{SM}}_{\Delta S=-2}(\mu)|K^0\rangle_{VSA} = 2\Big(\langle \bar{K}^0|\bar{s}_a\gamma^\mu(1-\gamma_5)d^a|0\rangle\langle 0|\bar{s}_b\gamma_\mu(1-\gamma_5)d^b|K^0\rangle$$

$$+ \langle \bar{K}^0|\bar{s}_a\gamma^\mu(1-\gamma_5)d^b|0\rangle\langle 0|\bar{s}_b\gamma_\mu(1-\gamma_5)d^a(x)|K^0\rangle\Big) , \qquad (3.59)$$

where repeated color indices are summed over and where the factor of 2 comes from the fact that the two factors of $(\bar{s}d)_{V-A}$ in $O^{\mathrm{SM}}_{\Delta S=-2}$ are interchangeable. Plugging (3.58) in (3.59) yields

$$\langle \bar{K}^0|O^{\mathrm{SM}}_{\Delta S=-2}(\mu)|K^0\rangle_{VSA} = \frac{2}{N_c^2} f_K^2 p^2 \left[\delta_a^a\delta_b^b + \delta_a^b\delta_b^a\right]$$

$$= 2\frac{N_c+1}{N_c} M_K^2 f_K^2 . \qquad (3.60)$$

This is clearly a rather crude approximation, as the LHS of Eq. (3.59) is μ dependent while the RHS is not. This approximation introduces a renormalization scale dependence which is unphysical.

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[8]Note that the K^0 does not actually decay leptonically: the $K^\pm$ do. However, in the isospin limit, the decay constant defined in Eq. (3.56) is equal to the physical decay constant f_K of the $K^\pm$.

A more modern approximation to the matrix element is obtained by keeping the leading term in a large-N_c expansion. The large-N_c, or 't Hooft limit ('t Hooft, 1974), is defined by taking $N_c \to \infty$ while holding $\alpha_s N_c$ fixed. By counting the number of α_s and loop factors of N_c in the various contributions to the relevant correlation functions (see below), it is straightforward to convince oneself that in the large-N_c limit, $B_K(\mu) = 3/4$. This corresponds to dropping the second term in Eq. (3.59), which is clearly suppressed by a factor of $1/N_c$ compared to the first. As in the VSA approximation $B_K(\mu)$ is μ independent, but here the μ dependence is also absent in the short-distance, Wilson coefficient, as can be seen by taking the large-N_c limit in Eqs. (3.44)–(3.51): the large-N_c approximation is a well-defined and self-consistent approximation scheme.

Before closing this section, it is worth mentioning that one can define a renormalization scheme and scale independent B-parameter, B_K^{RGI}, by multiplying $B_K(\mu)$ by $C(\mu)$ of Eq. (3.51) (with $N_c = 3$ and $N_f = 3$):

$$B_K^{\mathrm{RGI}} = C(\mu) \times B_K(\mu) . \tag{3.61}$$

3.4   Computation of bare B_K

On the lattice, the numerator of B_K is obtained from three-point functions. Quark propagators are given by:

$$S_q[\vec{x}, t; \eta, t_s; U] = \sum_{\vec{x}_s} D^{-1}[\vec{x}, t; \vec{x}_s, t_s; m_q; U] \eta(\vec{x}_s) , \tag{3.62}$$

where D is the lattice Dirac operator associated with the chosen fermion action, m_q the quark q's mass, U the gauge field configuration on which the propagator is computed, $\eta(\vec{x}_s)$ is a three dimensional source which may be a delta function or may have some spatial extent and t_s is the timeslice at which the source is placed. If only propagators from a point source at, for instance, $t_s = 0$ and $\vec{x}_s = \vec{0}$ (i.e. $\eta(\vec{x}_s) = \delta_{\vec{x}_s, \vec{0}}$), are available, then we can consider the following three-point function, in Euclidean spacetime of course:

$$C_3(t_i, t_f) = \sum_{\vec{x}_i, \vec{x}_f} \langle \bar{d}\gamma_5 s(\vec{x}_f, t_f) O_{\Delta S = -2}^{\mathrm{SM}}(0) \bar{d}\gamma_5 s(\vec{x}_i, t_i) \rangle , \tag{3.63}$$

where the argument of $O_{\Delta S = -2}^{\mathrm{SM}}$ is its spacetime position, not the renormalization scale. For $T/2 \gg -t_i \gg 1/\Delta E_K$ and $T/2 \gg t_f \gg 1/\Delta E_K$, $d\gamma_5 s(\vec{x}_i, t_i)$ creates a K^0 at $t = t_i$, this kaon then propagates to $t = 0$ where $O_{\Delta S = -2}^{\mathrm{SM}}(0)$ transforms it into a $\bar{K}^0$ and $\bar{d}\gamma_5 s(\vec{x}_f, t_f)$ destroys the resulting $\bar{K}^0$ at $t = t_f$. ΔE_K is the energy of the first excited state in the neutral kaon channel minus M_K. The sums over $\vec{x}_i$ and $\vec{x}_f$ put the initial and final kaons at rest. Thus, in this limit

$$C_3(t_i, t_f) \xrightarrow{T/2 \gg -t_i \gg 1/\Delta E_K, \, T/2 \gg t_f/ \gg 1/\Delta E_K} \frac{e^{-M_K(t_f - t_i)}}{4M_K^2} \langle 0|d\gamma_5 s(0)|\bar{K}^0(\vec{0})\rangle \tag{3.64}$$

$$\times \underbrace{\langle \bar{K}^0(\vec{0})|O_{\Delta S = -2}(0)|K^0(\vec{0})\rangle}_{\text{desired mat. elt.}} \langle K^0(\vec{0})|\bar{d}\gamma_5 s(0)|0\rangle .$$

This result is obtained by inserting a complete set of hadron states between $O_{\Delta S=-2}^{\text{SM}}(0)$ and $\bar{d}\gamma_5 s(\vec{x}_i, t_i)$, between $\bar{d}\gamma_5 s(\vec{x}_f, t_f)$ and $O_{\Delta S=-2}^{\text{SM}}(0)$ and between $\bar{d}\gamma_5 s(\vec{x}_i, t_i)$ and $\bar{d}\gamma_5 s(\vec{x}_f, t_f)$, keeping the sequence of states which gives rises to the smallest exponential suppression and which has the appropriate quantum numbers to give nonvanishing matrix elements. If $T/2 \gg t_f, -t_i$ is not realized, then contributions which are not significantly exponentially suppressed compared to the one in Eq. (3.64) will have to be added.

Similarly, to obtain the matrix elements required to construct the denominator of Eq. (3.55), we can consider the following two-point function

$$C_{2,\mu}(t) = \sum_{\vec{x}} \langle \bar{d}\gamma_5 s(\vec{x}, t) \bar{s}\gamma_\mu\gamma_5 d(0) \rangle \overset{t \gg \Delta_{E_K}}{\longrightarrow} \tag{3.65}$$

$$\frac{(e^{-M_K t} - e^{-M_K(T-t)})}{2M_K} \langle 0|d\gamma_5 s(0)|\bar{K}^0(\vec{0})\rangle \underbrace{\langle \bar{K}^0(\vec{0})|\bar{s}\gamma_5\gamma_\mu d(0)|0\rangle}_{\text{denom. mat. elt.}}, \tag{3.66}$$

where I have not assumed here that $T/2 \gg t$ to illustrate the additional contributions which arise in that case, and where I have used the properties of the correlation function under time reversal.

Then, B_K is obtained from the ratio

$$\frac{C_3(t_i, t_f)}{\sum_\mu C_{2,\mu}(t_f)C_{2,\mu}(t_i)} \overset{T/2 \gg -t_i \gg 1/\Delta E_K, \, T/2 \gg t_f/\gg 1/\Delta E_K}{\longrightarrow} B_K(a), \tag{3.67}$$

where I have reinstated $T/2 \gg t_f - t_i$ to get rid of "backward" contributions. In Eq. (3.67), the argument a of B_K is there to indicate that this is the value of B_K in the lattice regularized scheme and that it still requires renormalization.

To actually compute $C_3(t_i, t_f)$, we have to take the propagators of Eq. (3.62), contract them in the following way and average these contractions over the gauge ensemble, i.e.

$$C_3(t_i, t_f) = \frac{2}{\mathcal{N}_U} \sum_U \sum_{\vec{x}_i, \vec{x}_f} \left\{ \vphantom{\int} \right.$$

$$\underbrace{}_{\text{double trace term} \propto N_c^2}$$

$$\left. \vphantom{\int} \right\} , \qquad (3.68)$$

$$\underbrace{}_{\text{single trace term} \propto N_c}$$

where $\mathcal{N}_U$ is the number of independent gauge configurations. To get the time-reversed propagator required to construct the correlation function, one usually uses the γ_5 hermiticity which most lattice Dirac operators have,

$$S_d[\vec{0}, 0; \vec{x}, t; U] = \gamma_5 S_d[\vec{x}, t; \vec{0}, 0; U]^\dagger \gamma_5 . \qquad (3.69)$$

In Eq. (3.68), one clearly sees how, in the large-N_c limit, only the first contraction survives. The second contraction provides a $1/N_c$ suppressed correction. In practice, the two contractions have the same sign, and a cancellation operates in the calculation of B_K.

The method described above is actually a poor way to obtain B_K because the matrix elements of interest, $\langle \bar{K}^0(\vec{0}) | O_{\Delta S = -2}(0) | K^0(\vec{0}) \rangle$ and $\langle 0 | \bar{\gamma}_5 \gamma_\mu d(0) | K^0(\vec{0}) \rangle$, are sampled at only one point on the lattice: at the origin. We would gain a factor of roughly $(LM_\pi)^3$ in statistics if we could sample them over the whole three dimensional volume of the lattice. [9] Thus, a better way to calculate B_K is to have two zero momentum sources for the quark propagators, one at t_i and the other at t_f. One can consider, for instance, wall sources:

$$S_q[\vec{x}, t; W, t_W; U] = \sum_{\vec{x}_s} D^{-1}[\vec{x}, t; \vec{x}_s, t_W; m_q; U] \sum_{\vec{y}} \delta_{\vec{x}_s, \vec{y}} . \qquad (3.70)$$

Then, one constructs the following three-point function

$$C_3(t) = \frac{1}{N_U} \sum_U \sum_{\vec{x}} \gamma_5$$

$$\gamma_5 , \qquad (3.71)$$

---

[9]This is because the longest correlation length in the system is $1/M_\pi$ so that regions separated by that distance should be reasonably decorrelated.

where $t_i < 0$ and $t_f > 0$ are chosen so that there is a range of t around $t = 0$ such that the correlation function is dominated by the propagation of a zero momentum K^0 state between t_i and t and the propagation of a zero momentum $\bar{K}^0$ state between t and t_f. The gauge field configurations are usually gauge-fixed on the walls because wall sources correspond to meson sources and sinks of the form $\sum_{\vec{x},\vec{y}} \bar{d}_a(\vec{x}, t_W)\gamma_5 s^a(\vec{y}, t_W)$ which are clearly not gauge invariant, except for terms along the "diagonal" $\vec{x} = \vec{y}$. The gauge is usually fixed to Coulomb gauge. However, one can also not fix the gauge, the result being that the sums over the two quark positions in the sources and sinks reduce to a single diagonal sum over the positions after the average over gauge configurations is taken.

Using the wall sources, we also construct the two two-point functions $(t_W = t_i,\ t_f)$,

$$C_{2,\mu}(t, t_W) = \frac{1}{N_U} \sum_U \sum_{\vec{x}} \gamma_5 \quad \vec{x}, t \quad \gamma_\mu \gamma_5 \ . \tag{3.72}$$

Then we study the ratio of correlators

$$R(t) \equiv \frac{C_3(t)}{\sum_\mu C_{2,\mu}(t, t_f) C_{2,\mu}(t, t_i)} \tag{3.73}$$

as a function of t. For $t_i \ll t \ll t_f$, $R(t)$ develops a plateau (see Fig. 3.1) such that

$$R(t) \overset{t_i \ll t \ll t_f}{\longrightarrow} B_K(a) \ , \tag{3.74}$$

so that $B_K(a)$ is obtained by either averaging $R(t)$ or fitting it to a constant over the plateau region.

3.5 Renormalization of the Standard Model $|\Delta S| = 2$ operator

We are not done, however. As we already stated, simply inserting the lattice operator $O_{\Delta S=-2}^{\text{SM}}$ in $C_3(t)$ and computing $R(t)$ yields the bare $B_K(a)$. This quantity is divergent in the continuum limit and must be renormalized. And it must be done so in a renormalization scheme which matches the one used in the perturbative calculation of the short-distance Wilson coefficients.

It is straightforward to show that the full set of $\Delta S = -2$, $\Delta D = 2$ operators of dimension $d \leq 6$ can be written as:

$$O_1 = O_{\Delta S=-2}^{\text{SM}} = (\bar{s}d)_{V-A}(\bar{s}d)_{V-A} \qquad \text{(unmix)} \ , \tag{3.75}$$

$$O_{2,3} = (\bar{s}d)_{S-P}(\bar{s}d)_{S-P} \qquad \text{(unmix, mix)} \ , \tag{3.76}$$

$$O_{4,5} = (\bar{s}d)_{S-P}(\bar{s}d)_{S+P} \qquad \text{(unmix, mix)} \ , \tag{3.77}$$

where he subscripts $(\bar{s}d)_{S-P}$ and $(\bar{s}d)_{S+P}$ are defined in analogy with $(\bar{s}d)_{V-A}$ in Eq. (3.39). In Eqs. (3.75)–(3.77) "unmix" and "mix" refer to the color indices. In the "unmix" case, the color indices of the quark-antiquark pairs within parentheses are contracted; in the "mix" case, the color index of the quark of one pair is contracted

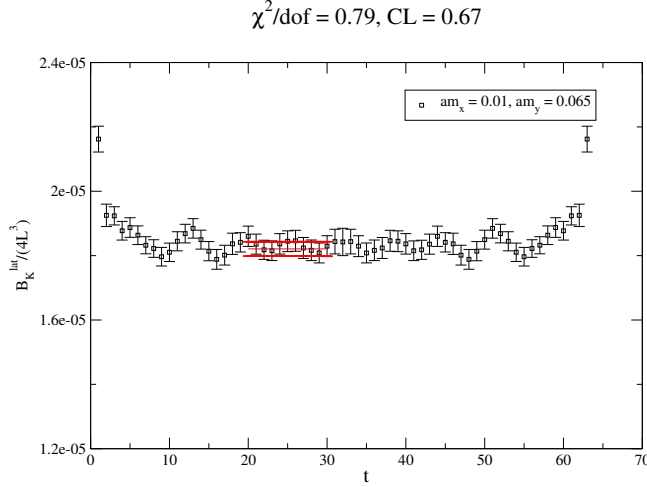$$\chi^2/\text{dof} = 0.79, \text{CL} = 0.67$$

Fig. 3.1 Plateau fit to $R(t)/(4L^3)$ on the coarse $N_f = 2 + 1$, staggered, MILC, $am_l/am_h = 0.007/0.05$ ensemble. The legend shows the nondegenerate pair of domain-wall, valence quark masses making up the kaon in the three-point correlation function. The correlated χ^2/dof and confidence level of the fit to a constant (red lines) are given in the title. Taken from (Aubin *et al.*, 2010).

with the color index of the antiquark of the other pair, and vice versa. Because O_1 Fierz transforms into itself, the "mix" and "unmix" O_1 are the same operator.

To understand the renormalization patterns of $O_{\Delta S=-2}^{\text{SM}}$ and the other $\Delta S = -2$ operators, it is useful to consider their transformation properties under various symmetry groups. Because we will only work in massless renormalization schemes, the $SU(3)_L \times SU(3)_R$ chiral group is a symmetry which is relevant here. Under the action of this group, $(\bar{s}d)_{V-A}(\bar{s}d)_{V-A}$ transforms in the $(27,1)$ representation, i.e. it is a 27 under $SU(3)_L$ and clearly a singlet under $SU(3)_R$, since it is composed only of left-handed fields. It is straightforward to derive the $SU(3)_L \times SU(3)_R$ representations to which the five $\Delta S = -2$ operators belong:

$$
\begin{aligned}
O_1 &\sim (27, 1) \xrightarrow{SU(3)_V} 27 \otimes 1 = 27 \,, \\
O_{2,3} &\sim (6, \bar{6}) \xrightarrow{SU(3)_V} 6 \otimes \bar{6} = 27 \oplus 8 \oplus 1 \,, \\
O_{4,5} &\sim (8, 8) \xrightarrow{SU(3)_V} 8 \otimes 8 = 27 \oplus 10 \oplus \overline{10} \oplus 8 \oplus 8 \oplus 1 \,.
\end{aligned}
\tag{3.78}
$$

In Eq. (3.78) I have also worked out the reduction of these representations to the diagonal, $V = L + R$, Eightfold Way, $SU(3)_V$ group, for reasons which will be clear shortly. Note that the "mix" versus "unmix" feature of these operators has no bearing on their flavor transformation properties as these features pertain solely to color.

From this, we see that $O_{\Delta S=-2}^{\text{SM}}$ is the only $\Delta S = -2 = -\Delta D$ operator of dimension 6 or less, which transforms as $(27,1)$. Thus, in any regularization which preserves $SU(3)_L \times SU(3)_R$ symmetry (or at least in the valence sector), $O_{\Delta S=-2}^{\text{SM}}$ renormalizes multiplicatively. This includes overlap and domain wall fermions, for sufficiently large

fifth dimension. Similarly, Eq. (3.78) indicates that the operator pairs (O_2, O_3) and (O_4, O_5) may mix within each pair under renormalization, but not with any of the other $\Delta S = -2 = -\Delta D$ operators.

The situation is very different for Wilson fermions. Indeed, the Wilson-Dirac operator breaks the chiral symmetry of continuum QCD explicitly, down to the vector flavor symmetry $SU(3)_V$. As Eq. (3.78) shows, $SU(3)_V$ is not sufficient to forbid $O_{\Delta S=-2}^{\mathrm{SM}}$ from mixing with the four other $\Delta S = -2 = -\Delta D$ operators, $O_{2,\cdots,3}$, under renormalization.

To push things further, we turn to parity. Since parity is preserved by Wilson fermions, we can consider separately the renormalization of the parity even and parity odd components of the operators. For B_K we are clearly interested in the parity even part:

$$\langle \bar{K}^0 | (\bar{s}d)_{V-A}(\bar{s}d)_{V-A} | K^0 \rangle = \langle \bar{K}^0 | (\bar{s}d)_V(\bar{s}d)_V + (\bar{s}d)_A(\bar{s}d)_A | K^0 \rangle . \qquad (3.79)$$

So let us begin with the renormalization of the parity even part.

At this point, it is useful to invoke a discrete symmetry transformation known as CPS (Bernard *et al.*, 1985). It consists in performing a CP transformation, followed by a switching $s \leftrightarrow d$. Note that this vector flavor symmetry is only softly broken by the mass terms in the action. Therefore, violations must appear multiplied by factors of $(m_s - m_d)$. Under CPS, we have:

$$\bar{s}\gamma^\mu d \xrightarrow{CPS} -\bar{s}\gamma_\mu d \qquad (3.80)$$

$$\bar{s}\gamma^\mu\gamma^5 d \xrightarrow{CPS} -\bar{s}\gamma_\mu\gamma^5 d \qquad (3.81)$$

$$\bar{s}d \xrightarrow{CPS} \bar{s}d \qquad (3.82)$$

$$\bar{s}\gamma^5 d \xrightarrow{CPS} -\bar{s}\gamma^5 d . \qquad (3.83)$$

Thus, the parity even components of the $\Delta S = -2$ operators transform under CPS as

$$O_1^+ = (\bar{s}d)_V(\bar{s}d)_V + (\bar{s}d)_A(\bar{s}d)_A \xrightarrow{CPS} O_1^+ , \qquad (3.84)$$

$$O_{2,3}^+ = (\bar{s}d)_S(\bar{s}d)_S + (\bar{s}d)_P(\bar{s}d)_P \xrightarrow{CPS} O_{2,3}^+ , \qquad (3.85)$$

$$O_{4,5}^+ = (\bar{s}d)_S(\bar{s}d)_S + (\bar{s}d)_P(\bar{s}d)_P \xrightarrow{CPS} O_{4,5}^+ . \qquad (3.86)$$

All of these operators are CPS eigenstates, with eigenvalue $+1$. Like $SU(3)_V$ symmetry, CPS does not forbid O_1^+ to mix with $O_{2,\cdots,3}^+$, under renormalization. In fact, there is no symmetry which forbids O_1^+ to mix with the other operators and one finds, in practice, that they do mix. We have,

$$O_1^+(\mu) = Z_1^+(a, \mu)\left[O_1^+(a) + \sum_{i=2}^{5} z_{1i}(a)O_i^+(a)\right] , \qquad (3.87)$$

where $Z_1^+(a, \mu)$ is logarithmically divergent in the continuum limit, while the mixing factors, $z_{1i}(a)$, are finite (Testa, 1998). Using the fact that the values of B_K^{RGI}

of Eq. (3.61), obtained in the continuum renormalization scheme and in the lattice regularization scheme, must be identical, one easily obtains a formal expression for the renormalization constant $Z_1^+(a, \mu)$, to all orders in perturbation theory:

$$Z_1^+(a, \mu) = \exp \left\{ \int_0^{a_s(\mu)} \frac{da_s}{a_s} \frac{\gamma(a_s)}{\beta(a_s)} - \int_0^{a_s^{\text{lat}}} \frac{da_s}{a_s} \frac{\gamma^{\text{lat}}(a_s)}{\beta^{\text{lat}}(a_s)} \right\} \ , \qquad (3.88)$$

with $a_s^{\text{lat}} = g_0^2/(4\pi)^2$, where g_0 is the bare lattice coupling. Expansions in the bare lattice coupling are notoriously poorly behaved, and one can usually improve their convergence by expressing them in terms of a renormalized continuum coupling, such as $a_s(\mu)$ at $\mu = 1/a$ for example. Applying this to Eq. (3.88), we find

$$Z_1^+(a, \mu) = \exp \left\{ \int_0^{a_s(\mu)} \frac{da_s}{a_s \beta(a_s)} \gamma(a_s) - \int_0^{a_s(1/a)} \frac{da_s}{a_s \beta(a_s)} \bar{\gamma}^{\text{lat}}(a_s) \right\} \ , \qquad (3.89)$$

where $\bar{\gamma}^{\text{lat}}$ is the anomalous dimension obtained by rewriting γ^{lat} in terms of the continuum coupling a_s. Obviously this change of variable would make no difference to $Z_1^+(a, \mu)$ were it to be computed to all orders in perturbation theory. However, at finite order this reordering of the expansion may improve the convergence of the series.

It is interesting to expand Eq. (3.89) to one loop–this could be done for Eq. (3.88) instead–to explicitly see the relationship between the coefficients of the expansion and the anomalous and beta function coefficients. We find:

$$Z_1^+(a, \mu) = 1 - \frac{\alpha_s}{4\pi} \left(\gamma_0 \ln(a\mu)^2 + \frac{\bar{\gamma}_1^{\text{lat}} - \gamma_1}{\beta_0} \right) + O(\alpha_s^2) \ . \qquad (3.90)$$

One clearly sees that the constant $O(a_s)$ term knows about the two-loop anomalous dimension (it is a subleading log) whereas the leading log term is given by γ_0. At this same order, the mixing coefficients are finite and given by

$$z_{1i}(a) = z_{1i}^{(1)} \frac{\alpha_s}{4\pi} + O(\alpha_s^2) \qquad i = 2, \cdots, 5 \ , \qquad (3.91)$$

where the $z_{1i}^{(1)}$ are constants.

Now, the $SU(3)_L \times SU(3)_R$ properties of the operators indicate that the physical contributions in $\langle \bar{K}^0|O_1^+(a)|K^0\rangle$ are chirally suppressed compared to the nonphysical ones: $O(p^2)$ vs $O(1)$ in χPT counting. Thus, even though the mixing of O_1 with $O_2,\ldots,O_5$ is α_s suppressed, this suppression can easily be compensated by an $O(10 - 20)$ enhancement from the matrix element (Babich *et al.*, 2006). This means that the necessary subtractions are delicate and it is preferable to avoid calculating B_K with Wilson fermions.

It is also interesting to study the transformation properties of the parity odd components of $O_1, \cdots, O_5$ under CPS. We find

$$O_1^- = -2(\bar{s}d)_V(\bar{s}d)_A \xrightarrow{CPS} O_1^- \qquad (3.92)$$

$$O_{2,3}^- = -2(\bar{s}d)_S(\bar{s}d)_P \xrightarrow{CPS} -O_{2,3}^- \qquad (3.93)$$

$$O_{4,5}^- = 0 \ . \qquad (3.94)$$

Thus, CPS forbids O_1^- to mix with $O_{2,3}^-$ and $O_{4,5}^-$ vanish anyway. We conclude that O_1^-, unlike O_1^+, renormalizes multiplicatively:

$$O_1^-(\mu) = Z_1^-(a,\mu)O_1^-(a) \ . \tag{3.95}$$

This turns out to be useful for twisted-mass QCD (tmQCD), which is described in detail in (Vladikas, 2010). For instance, twisting (u, d) by an angle α and leaving the strange quark s untwisted, we have

$$[O_{VV+AA}]_{\text{QCD}} \equiv [(\bar{s}d)_V(\bar{s}d)_V + (\bar{s}d)_A(\bar{s}d)_A]_{\text{QCD}}$$
$$= \cos\alpha \, [O_{VV+AA}]_{\text{tmQCD}} - i\sin\alpha \, [O_{VA+AV}]_{\text{tmQCD}} \ . \tag{3.96}$$

So, picking $\alpha = \pi/2$ (i.e. maximal twist), the above equation implies the following relationship between the renormalized matrix elements:

$$\langle \bar{K}^0 | O_{VV+AA}(\mu) | K^0 \rangle_{\text{QCD}} = -i\langle \bar{K}^0 | O_{VA+AV}(\mu) | K^0 \rangle_{\text{tmQCD}} \ . \tag{3.97}$$

Then, since CPS symmetry is only softly broken in tmQCD, $\langle \bar{K}^0 | O_{VA+AV}(a) | K^0 \rangle_{\text{tmQCD}}$ renormalizes multiplicatively. [10] Thus, by working in tmQCD at maximal twist, one can compute $B_K(\mu)$ performing only multiplicative renormalization (please see Tassos' course notes (Vladikas, 2010) for details).

Though we discussed renormalization mostly in terms of perturbation theory, I greatly encourage you to perform this renormalization nonperturbatively, with one of the methods explained in Peter (Weisz, 2010) or Tassos' (Vladikas, 2010) course notes. You may also want to look into the renormalization procedure put forward in (Dürr *et al.*, 2010*a*; Dürr *et al.*, 2010*b*), which enhances the RI/MOM method of (Martinelli *et al.*, 1995) with nonperturbative, continuum running (see also (Arthur and Boyle, 2010)). Or if you choose to renormalize perturbatively, you should at least do so to two loops to ensure that you have some control over the perturbative series. Of course, one may argue that the short distance coefficients in Eq. (3.41) are only known to NLO, and that there is no point in doing much better in the lattice to continuum matching. Moreover, there are other uncertainties in the relation (3.22) of ϵ to B_K, such as the one associated with the error on the determination of $|V_{cb}|$ or with the neglect of $1/m_c^2$ and of the $\text{Im}A_0/\text{Re}A_0$ corrections (see e.g. (Lellouch, 2009)). However, it is admittedly a pity to perform a careful nonperturbative computation of the bare matrix elements only to introduce perturbative uncertainties through the matching procedure.

3.6   Final words on K^0-$\bar{K}^0$ mixing

Given a preferably nonperturbatively renormalized B_K, it must be matched to the scheme used in the computation of the Wilson coefficients which appear in Eq. (3.41), and computed for a variety of lattice spacings and quark masses. Then you must use

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[10]CPS violating terms are proportional to $(m_s - m_d)$, so that $O_{VV+AA}(a)$ can only mix with higher dimensional operators which are suppressed by powers of the lattice spacing and the latter can only contribute discretization errors.

the methods described in, for instance, (Dürr *et al.*, 2008; Lellouch, 2009; Dürr *et al.*, 2010*a*; Dürr *et al.*, 2010*b*) and/or in Pilar (Hernández, 2010), Peter (Weisz, 2010) and Maarten's (Golterman, 2010) course notes to extrapolate (preferably interpolate) to the physical values of m_{ud}, m_s and extrapolate to the continuum limit. Finally, you must perform a complete systematic error analysis, such as the ones performed in (Dürr *et al.*, 2008; Dürr *et al.*, 2010*c*; Dürr *et al.*, 2010*a*; Dürr *et al.*, 2010*b*). For a recent, comprehensive review of lattice calculations of B_K, see for instance (Colangelo *et al.*, 2010).

Before concluding this discussion of K^0-$\bar{K}^0$ mixing, it is worth mentioning that lattice QCD can also provide information that is relevant for this process beyond the Standard Model. Quite generically, when one adds heavy degrees of freedom to those of the Standard Model, such as in supersymmetric extensions, one finds that the full set of $\Delta S = -2$ operators of Eqs. (3.75)–(3.77) contribute to the low-energy effective Hamiltonian. Of course, the lattice can also be used to compute the matrix elements of the four additional operators, between K^0 and $\bar{K}^0$ states. This has been studied in the quenched approximation in (Donini *et al.*, 1999; Babich *et al.*, 2006). Ref. (Babich *et al.*, 2006) finds ratios of non Standard Model to Standard Model matrix elements which are roughly twice as large as those in (Donini *et al.*, 1999). As explained in (Babich *et al.*, 2006), this is most probably due to discretization errors present in (Donini *et al.*, 1999). This picture appears to be confirmed by the preliminary $N_f = 2$ results of (Dimopoulos *et al.*, 2010).

3.7 Phenomenology of the $\Delta I = 1/2$ rule

The goal here is to compute nonleptonic weak decay amplitudes, such as those for $K \to \pi\pi$, directly in the Standard Model, without any extraneous model assumptions, nor potentially uncontrolled approximations such as LO, $SU(3)$ χPT. This is critical for showing that QCD is indeed responsible for surprising phenomena such as the $\Delta I = 1/2$ rule, or deciding whether New Physics is hidden in the experimental measurement of direct CP violation in $K \to \pi\pi$ (i.e. of ϵ'). In the following I will concentrate on the $\Delta I = 1/2$ rule as the calculation of ϵ' is significantly more difficult. For the latter, the renormalization of the relevant matrix elements is more complicated (Dawson *et al.*, 1998). There are more matrix elements involved and there appear to be important cancellations between them (see e.g. (Buchalla *et al.*, 1996)). Moreover, final-state interactions, such as the ones discussed in (Pallante and Pich, 2001; Buras *et al.*, 2000), seem to play an important role. Indeed, recent attempts to exhibit the $\Delta I = 1/2$ rule and to determine $\mathrm{Re}(\epsilon'/\epsilon)$ using soft pion theorems appear to fail due to the large chiral corrections required to translate the $K \to \pi$ and $K \to 0$ amplitudes computed on the lattice into physical $K \to \pi\pi$ amplitudes (Li and Christ, 2008; Sachrajda, 2010*a*; Christ, 2010*a*).

Experimentally, the partial widths measured in the different $K \to \pi\pi$ decay channels, together with the corresponding isospin changes between the final two-pion and initial kaon states, are (Nakamura *et al.*, 2010):

$$\Gamma_{+-} = \Gamma(K_S \to \pi^+\pi^-) = 5.08 \times 10^{-12} \text{MeV} \qquad \Delta I = \frac{1}{2}, \frac{3}{2} \qquad (3.98)$$

$$\Gamma_{00} = \Gamma(K_S \to \pi^0\pi^0) = 2.26 \times 10^{-12} \text{MeV} \qquad \Delta I = \frac{1}{2}, \frac{3}{2} \qquad (3.99)$$

$$\Gamma_{+0} = \Gamma(K^+ \to \pi^+\pi^0) = 1.10 \times 10^{-14} \text{MeV} \qquad \Delta I = \frac{3}{2} . \qquad (3.100)$$

Using these results, we find

$$\frac{\Gamma_{+-}}{\Gamma_{+0}} = 463. \quad \text{and} \quad \frac{\Gamma_{00}}{\Gamma_{+0}} = 205. , \qquad (3.101)$$

whereas Γ_{+-}/Γ_{+0} should be ~ 1 in the electroweak theory and in the absence of the strong interaction. Now, in terms of the amplitudes, the rates are

$$\Gamma_{+-} = \frac{\gamma}{3} \left[2|A_0|^2 + |A_2|^2 + 2\sqrt{2}\text{Re}\left(A_0 A_2^* e^{i(\delta_0 - \delta_2)} \right) \right] , \qquad (3.102)$$

$$\Gamma_{00} = \frac{\gamma}{3} \left[|A_0|^2 + 2|A_2|^2 - 2\sqrt{2}\text{Re}\left(A_0 A_2^* e^{i(\delta_0 - \delta_2)} \right) \right] , \qquad (3.103)$$

$$\Gamma_{+0} = \frac{3}{4}\gamma|A_2|^2 , \qquad (3.104)$$

with $\gamma = \sqrt{M_K^2 - 4M_\pi^2}/(16\pi M_K^2)$. Considering $\Gamma_{+-} + \Gamma_{00}$ and Γ_{+0}, and taking $M_\pi = 134.8.$ MeV and $M_K = 494.2$ MeV (i.e. isospin limit values), we find

$$|A_0| = 4.66 \times 10^{-4} \text{ MeV} \quad \text{and} \quad |A_2| = 2.08 \times 10^{-5} \text{ MeV} \qquad (3.105)$$

$$\to \frac{|A_0|}{|A_2|} = 22.4 , \qquad (3.106)$$

whereas the combined chiral and large-N_c limit predicts $\sqrt{2}$ (Lellouch, 2001)! It is the huge enhancement of over 400 in the rate or 20 in the amplitude which is known as the $\Delta I = 1/2$ enhancement. It was termed a "rule" because this enhancement of $\Delta I = 1/2$ over $\Delta I = 3/2$ transitions is also observed in other decays, such as $\Lambda \to N\pi$, $\Sigma \to N\pi$ and $\Xi \to \Lambda\pi$.

3.8 The $\Delta I = 1/2$ rule in the Standard Model

At leading order in the weak and strong interactions, $\Delta S = -1$, $\Delta D = 1$ transitions occur through the tree level diagram
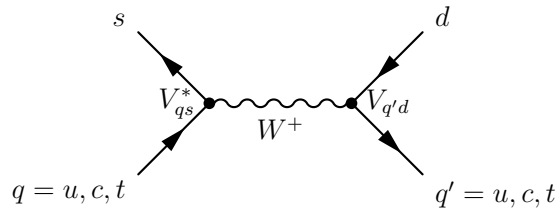
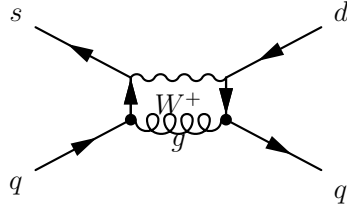As usual, we integrate out the heavy W boson and t quark. At leading order in QCD, this yields the following four-quark, local vertex

$$\longrightarrow \frac{G_F}{2\sqrt{2}} \sum_{q,q'=u,c} V_{q'd}V_{qs}^* Q_2^{qq'}$$

with

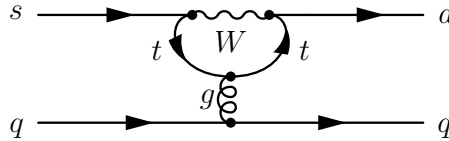$$Q_2^{qq'} = (\bar{s}q)_{V-A}(\bar{q}'d)_{V-A} \ . \tag{3.107}$$

Now, if we include α_s corrections (Gilman and Wise, 1979), such as

we generate a new operator:

$$Q_1^{qq'} = (\bar{s}d)_{V-A}(\bar{q}'q)_{V-A} \ . \tag{3.108}$$

These corrections also lead to the penguin diagram

with $q = u, d, s, c, b$. However, one finds that they yield tiny contributions to the CP conserving parts of $K \to \pi\pi$ decays. Thus, we neglect these here. Moreover, we are only interested in external states with u, d and/or s quarks. So we do not need operators with a single charm leg. To simplify the operator structure, we can also use the unitarity of the CKM matrix:

$$V_{cd}V_{cs}^* = -V_{ud}V_{us}^* - V_{td}V_{ts}^* \ , \tag{3.109}$$

where the second term on the RHS of this equation can be neglected because it is multiply Cabibbo suppressed by a factor of $\lambda^4 \sim 0.003$ compared to the first term. Then, for CP conserving $\Delta S = -1$, $\Delta D = 1$ transitions, we have the effective Hamiltonian

$$\mathcal{H}_{\text{CPC}}^{\Delta S=-1} = \frac{G_F}{\sqrt{2}} V_{ud}V_{us}^* \sum_{i=\pm} C_i(\mu)O_i \tag{3.110}$$

with

$$O_\pm = [(\bar{s}u)_{V-A}(\bar{u}d)_{V-A} \pm (\bar{s}d)_{V-A}(\bar{u}u)_{V-A}] - [u \to c] \ , \tag{3.111}$$

where the second term, in which u is replaced by c with an overall minus sign, implements the GIM suppression mechanism (Glashow *et al.*, 1970). It is straightforward

to show that O_+ is in the $(84, 1)$ representation of the $SU(4)_L \times SU(4)_R$ chiral group, appropriate for classifying operators composed of u, d, s and c quarks for renormalization in massless schemes: it is a completely symmetric and traceless tensor in two fundamental and two conjugate $SU(4)_L$ indices. O_-, on the other hand, is in the $(20, 1)$ representation of this group (it is a completely antisymmetric and traceless tensor in two fundamental and two conjugate $SU(4)_L$ indices). Thus, O_+ and O_- do not mix under renormalization. In Eq. (3.110), the short distance Wilson coefficients are given, at $O(\alpha_s)$, by (Gaillard and Lee, 1974a; Altarelli and Maiani, 1974; Altarelli *et al.*, 1981):

$$C_\pm(\mu) = 1 + \frac{\alpha_s}{4\pi} \left(\gamma_\pm^{(0)} \ln \frac{\mu^2}{M_W^2} + \delta_\pm \right) \ , \tag{3.112}$$

with, in the $\overline{\text{MS}}$-NDR scheme:

$$\gamma_\pm^{(0)} = \pm 3 \frac{N_c \mp 1}{N_c} \quad \text{and} \quad \delta_\pm = \pm \frac{11}{2} \frac{N_c \mp 1}{N_c} \ . \tag{3.113}$$

One often pushes the short distance calculation further and integrates out the charm quark. But the GIM mechanism is very useful for reducing the divergences of relevant weak matrix element on the lattice. (Unfortunately, we will not have the time to cover this here, but I refer the interested reader to (Dawson *et al.*, 1998), for instance, for a discussion of this and related issues.)

A straightforward analysis of the isospin structure of the operators of Eq. (3.111) show that O_- is pure $I = \frac{1}{2}$, while O_+ has both $I = \frac{1}{2}$, $\frac{3}{2}$ components. [11] One may wonder then, whether the $\Delta I = 1/2$ enhancement comes from the running of the Wilson coefficients $C_\pm(\mu)$ from the scale $\mu \sim M_W$, where the ratio $C_-(\mu)/C_+(\mu)$ is 1 plus small corrections of order $\alpha_s(M_W) \sim 0.1$, down to a scale $\mu \sim 2\,\text{GeV}$. This would mean that the $\Delta I = 1/2$ rule could be understood as a short-distance enhancement. At leading-log order (LL) (Gaillard and Lee, 1974a; Altarelli and Maiani, 1974), using Eq. (3.50), we find $C_-(2\,\text{GeV})/C_+(2\,\text{GeV}) = (\alpha_s(2\,\text{GeV})/\alpha_s(m_b))^{18/25}$ $(\alpha_s(m_b)/\alpha_s(M_W))^{18/23}$ $(C_-(M_W)/C_+(M_W)) \sim 2$. So there is some short-distance enhancement, but not enough by a long shot to explain the $\Delta I = 1/2$ rule. [12] In turn, this means that most of the enhancement in

$$\left| \frac{A_0}{A_2} \right| = \frac{\langle (\pi\pi)_0 | C_+ O_+ + C_- O_- | K^0 \rangle}{\langle (\pi\pi)_2 | C_+ O_+ | K^0 \rangle} \tag{3.114}$$

must come from long distances.

One may also wonder what role the charm quark plays in these decays. In particular, one might consider an imaginary world in which the GIM mechanism is exact, i.e. $m_c = m_u$. Does the $\Delta I = 1/2$ enhancement persist in that limit? One way to

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[11] In terms of $SU(3)_L \times SU(3)_R$ representations, O_- is pure $(8, 1)$ while O_+ contains both $(8, 1)$ and $(27, 1)$ representations.

[12] If you have been reading these notes carefully, you will be quick to point out that this statement has its limitations. Indeed, beyond LLO, the running of the Wilson coefficients is scheme dependent. However, it is difficult to justify not going beyond that order at scales $\mu \sim 2\,\text{GeV}$. So the statement should be be understood as applying to commonly used schemes.

address this problem is to work in the $SU(4)$ chiral limit and determine the LECs corresponding to O_- and O_+, i.e. the $(20, 1)$ and $(84, 1)$ couplings (see comments after Eq. (3.111)) (Giusti *et al.*, 2007). Numerically, in the quenched approximation, it is found that there is an enhancement of $|A_0/A_2|$ over naive expectation (e.g. large-N_c), but that this enhancement is roughly a factor of four too small.

An interesting way to understand this $SU(4)$ chiral limit enhancement is to consider the three-point function contractions required to determine the matrix elements $\langle \pi^+|O_\pm|K^+\rangle$. It is straightforward to see that in the case of O_+, with the appropriate flavor replacements, the contractions are the same as those of Eq. (3.68), up to the overall factor of 2. On the other hand, for the pure $\Delta I = 1/2$ operator O_-, the contractions are those Eq. (3.68), but with a plus sign between the double and single trace terms. Thus, in the large-N_c limit, the two matrix elements coincide and we find the value of $|A_0/A_2| = \sqrt{2}$ discussed after Eq. (3.106). However, for finite N_c, the single trace term contributes, and does so with opposite signs to $\langle \pi^+|O_+|K^+\rangle$ and to $\langle \pi^+|O_-|K^+\rangle$. Since both trace contractions are positive, the larger the single trace term, the larger is $\langle \pi^+|O_-|K^+\rangle$ and the smaller is $\langle \pi^+|O_+|K^+\rangle$. This creates a $\Delta I = 1/2$ enhancement in which both the numerator $|A_0|$ is enhanced and the denominator $|A_2|$ is depressed. The argument also implies an anticorrelation between B_K, the B-parameter of K^0-$\bar{K}^0$ mixing, and the $\Delta I = 1/2$ enhancement of $|A_0/A_2|$. Indeed, in the chiral limit, the smaller B_K is compared to its large-N_c value of $3/4$, the larger $|A_0/A_2|$ is compared to $\sqrt{2}$, as first noted in (Pich and de Rafael, 1996).

Given the argument which we made earlier, one would think that LQCD is well suited to study $K \to \pi\pi$ decays. However, there are many conceptual problems one encounters when trying to study these decays on the lattice. Some of these are:

- The renormalization of the $\Delta S = -1$ effective Hamiltonian is difficult on the lattice, even more so for the CP violating part (see e.g. (Dawson *et al.*, 1998));
- lattices are only a few fermi in size and the final-state hadrons cannot be separated into isolated, asymptotic states;
- only approximately evaluated Euclidean correlation functions are available

There are also technical challenges. For instance, the study of these decays requires the calculation of 4-point functions. Moreover, power divergences must be subtracted, if the charm quark is integrated out in the case of CP conserving decays, and once the W and t are integrated out in the CP violating case. Both these points make the study of $K \to \pi\pi$ decays very demanding numerically.

3.9 Euclidean correlation functions and the Maiani-Testa theorem

For well over a decade, it was believed that $K \to \pi\pi$ amplitudes could not be studied directly on the lattice. Indeed, these amplitudes have both real and imaginary strong-interaction contributions while, in the Euclidean, correlation functions are purely real (or imaginary). Thus, it was difficult to see how such amplitudes could be extracted from a lattice calculation, necessarily performed in the Euclidean.

Of course, the Osterwalder-Schrader theorem (Osterwalder and Schrader, 1973; Osterwalder and Schrader, 1975) guarantees that Euclidean correlation functions can

be continued to Minkowski space, at least in principle. However, in practice such analytical continuations are essentially impossible with approximate Euclidean results.

This led Maiani and Testa, in 1990, to investigate what can be extracted from Euclidean correlation functions without analytical continuation (Maiani and Testa, 1990). They considered the following type of center-of-mass frame Euclidean correlation function,

$$\langle \pi(\vec{p}, t_1) \pi(-\vec{p}, t_1) \mathcal{H}_{\text{eff}}^{\Delta S = -1} K^\dagger(\vec{0}, t_i) \rangle \; , \tag{3.115}$$

and asked the question: what information does this correlation function contain regarding physical $K \to \pi\pi$ decay amplitudes in the usual lattice, asymptotic limit, i.e. $t_1, t_2 \gg 1/M_\pi$, $-t_i \gg 1/M_K$?

To "simplify" the problem and disentangle Euclidean from other possible lattice effects, they chose to work in a large, quasi-infinite volume. This apparently innocuous assumption has rather important consequences. For one, in infinite volume, the $\pi\pi$ spectrum is continuous. This means that in the limit $-t_i \gg 1/M_K$ and $t_1, t_2 \gg 1/M_\pi$, only the ground state contribution can be picked out: there is no known numerical technique to isolate an excited state in a continuous spectrum. In turn, this implies that one can only extract information about the matrix element $\langle \pi(\vec{0})\pi(\vec{0})|\mathcal{H}_{\text{eff}}^{\Delta S = -1}|K(\vec{0})\rangle$, in which all mesons are at rest: the physical decay is not directly accessible on the lattice.

This statement became known as the "Maiani-Testa theorem." It was a formalization of the general belief that $K \to \pi\pi$ decays could not be studied directly on the lattice but rather that approximations (Bernard *et al.*, 1985) or models (Ciuchini *et al.*, 1996) were needed to obtain information about physical $K \to \pi\pi$ decays from lattice calculations.

However, as is often the case with "no-go" theorems, the solution is found by questioning the underlying, apparently innocent assumptions. Here, it was the infinite volume assumption that brought in all of the difficulties while, for simulations performed in boxes with sides of a few fermi at most, it does not even approximately hold.

3.10 Two-pion states in finite volume

In a finite box with sides L, [13] two pions cannot be isolated into noninteracting asymptotic states. Rather, the $\pi\pi$ eigenstates are the result of a stationary scattering process. In addition, boundary conditions generically imply that the particles' momenta are quantized. For periodic boundary conditions, they come in discrete multiples of $2\pi/L$: $\vec{k} = \vec{z}(2\pi/L)$, with $\vec{z} \in \mathbb{Z}^3$. In turn, this means that the spectrum is discrete and the splitting is actually rather large for box sides of a few fermi. In such boxes, the typical spacing between momenta is $\Delta p = 2\pi/L = 1.2\,\text{GeV}/L[\text{fm}]$. This is clearly quite different from the continuous spectrum found in infinite volume.

In the free theory, in the center-of-mass frame and in the A_1^+ (i.e. cubic spin-0) sector, the energy of the n-th excited state is given by:

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[13]L must be large enough so that the range of the interaction between the two pions is contained within the box.
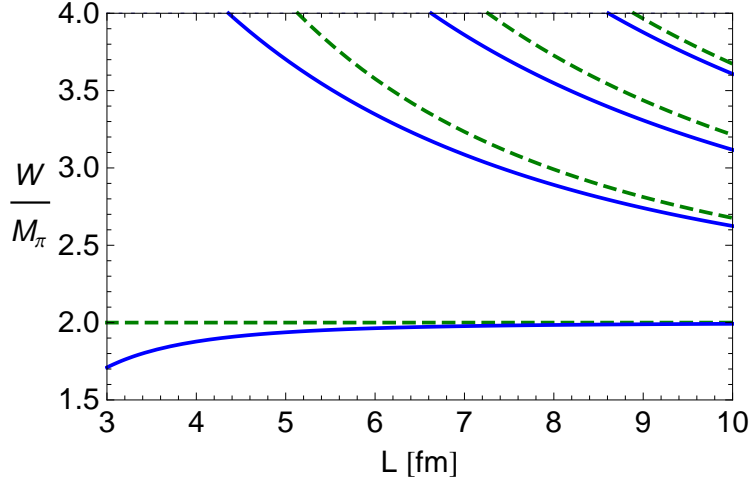
Fig. 3.2 The two-pion spectrum in a box of volume L^3 as a function of L in the $I = J = 0$ channel, under the four-pion threshold $W/M_\pi = 4$. The free spectrum is depicted by the green dashed curves. The solid blue curves show the interacting spectrum as obtained from Eq. (3.121), using the one-loop $I = J = 0$ phase shift from (Gasser and Meissner, 1991; Knecht *et al.*, 1995).

$$W_n^{(0)} = 2\sqrt{M_\pi^2 + n\left(\frac{2\pi}{L}\right)^2} \, , \tag{3.116}$$

for $n \leq 6$–there is no integer three-vector with norm squared, 7, nor 8 for that matter. This spectrum is shown as the dashed lines in Fig. 3.2.

In the presence of interactions, the energy W_n of the fully interacting state was worked out by Martin to all orders in relativistic quantum field theory (Lüscher, 1986; Lüscher, 1991) for two-pion energies below the four-pion threshold, up to corrections which fall of exponentially with the box size (i.e. up to finite-volume, vacuum polarization effects).

The ground state $n = 0$ requires special treatment. In the isospin $I = 0$ and spin $J = 0$ channel, we have (Lüscher, 1986):

$$W_0 = 2M_\pi - \frac{4\pi a_I}{M_\pi L^3}\left\{1 + c_1\frac{a_I}{L} + c_2\left(\frac{a_I}{L}\right)^2\right\} + O(L^{-6}) \tag{3.117}$$

where

$$c_1 = -2.837297, \qquad c_2 = 6.375183 \, , \tag{3.118}$$

where the S-wave scattering length in the appropriate channel is a_I with

$$a_I = \lim_{k\to 0}\frac{\delta_I(k)}{k} \, , \tag{3.119}$$

and where k is the momentum of the pions in the center-of-mass frame.

For excited states, the results are given in terms of the scattering phase, δ_I, of the relevant isospin channel. The appearance of scattering phases should not be surprising. We know from scattering theory that, under reasonable conditions, potentials can be reconstructed from these phases. Martin finds that (Lüscher, 1991)

$$W_n = 2\sqrt{M_\pi^2 + k_n^2} \qquad n = 1, 2, 3, \dots \ , \tag{3.120}$$

where k_n is a solution of the quantization equation

$$n\pi - \delta_I(k_n) = \phi(q_n) \ , \tag{3.121}$$

with $q_n \equiv k_n L/(2\pi)$ and with

$$\tan \phi(q) = -\frac{\pi^{3/2} q}{Z_{00}(1; q^2)} \ . \tag{3.122}$$

$\phi(q)$ is defined for $q \geq 0$. It is such that $\phi(0) = 0$ and it depends continuously on q. It is given in terms of the zeta function of the Laplacian

$$Z_{00}(s; q^2) = \frac{1}{\sqrt{4\pi}} \sum_{\vec{n} \in \mathbb{Z}^3} \left(\vec{n}^2 - q^2 \right)^{-s} \ , \tag{3.123}$$

for Re $s > 3/2$ and by analytic continuation elsewhere. A useful integral representation for evaluating $Z_{00}(1; q^2)$ numerically is given in Sec. 4.

Solving Eq. (3.121), one generically finds

$$W_n = 2\sqrt{M_\pi^2 + n\left(\frac{2\pi}{L}\right)^2} + O\left(\frac{1}{L^3}\right) \ , \tag{3.124}$$

where the equation actually gives the whole tower of $1/L$ corrections once the scattering phase is specified. As already stated, the equation holds for $n \leq 6$ and there is no integer three-vector whose squared norm is 7 or 8. Then, beginning at 9, there are integer vectors, $\vec{z}$, which are not related by cubic rotations but which have the same squared norm, e.g. $\vec{z_1} = (2, 2, 1)$ and $\vec{z_2} = (3, 0, 0)$. In a treatment where only the $O(3)$ spin-0 component of the A_1^+ representation is taken into account [14], the states associated with such three-vectors in the free case do not feel the interaction in the interacting case either, and have $k = |\vec{z}|(2\pi/L)$. This is because they combine into states with $O(3)$ spin-4 and/or higher spins. Such states will be ignored in the following and we will consider only $n \leq 6$, which is certainly not a limitation in practice.

The full solution (taking for instance $I = J = 0$) is shown in Fig. 3.2. The first remark which can be made is that the two-pion spectrum on lattices which can be considered in the foreseeable future is far from being continuous. The second is that distortions due to interactions are quite small: the volume suppression of the corrections is effective when $L \geq 3\,\text{fm}$. Finally, it is clear that by studying the energies $W_n(L)$

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[14]Because the cube is not invariant under generic rotations, the irreducible representations of the cubic group are resolved into many irreducible representations of $O(3)$. For the A_1^+ cubic representation, the relevant spin representations are spin 0, 4,....

as a function of box size L, we can turn Eq. (3.121) around and reconstruct, at least for a few discrete momenta, the scattering phase $\delta_I(k)$.

Now, suppose that there is a single resonance R in this $\pi\pi$ channel, with mass $M_R < 4M_\pi$, i.e. under the inelastic threshold, and width Γ_R. To explain how Martin's equation works in that case, it is useful to turn to quantum mechanics. A quantum mechanics approach is actually justified because corrections suppressed exponentially in L are neglected in the derivation of the quantization formula. Such suppression factors generically correspond to tunneling phenomena. Here they are associated with features of relativistic quantum field theories which are absent in quantum mechanics: the exchange of a virtual particle around the box.

We begin by decomposing the total Hamiltonian H of the two-pion system into a free part H_0 and an interaction H_{int}:

$$H = H_0 + H_{int} \ . \tag{3.125}$$

Then we consider the n-th free $\pi\pi$ state ($n \leq 6$), $|n_0\rangle$, in our chosen channel (here isospin $I = 0$ or 2 and $J^p = 0^-$). It is such that $\langle n_0|n_0\rangle = 1$ and

$$H_0|n_0\rangle = W_n^{(0)}|n_0\rangle \ . \tag{3.126}$$

To understand what this energy becomes in the presence of interactions and of the resonance, it is useful to consider a perturbative expansion in the interaction H_{int}, though the final result is accurate to all orders. Denoting the resulting energy W_n, and $|n\rangle$, the corresponding fully-interacting eigenstate, we have, to second order in H_{int}:

$$
\begin{aligned}
W_n &= \langle n|H|n\rangle \\
&= W_n^{(0)} + \langle n_0|H_{int}|n_0\rangle + \sum_\alpha \frac{\langle n_0|H_{int}|\alpha\rangle\langle\alpha|H_{int}|n_0\rangle}{W_n^{(0)} - W_\alpha} + \cdots \ .
\end{aligned}
\tag{3.127}
$$

Here α runs over 2, 4, ... pion states, as well as any other state which appears in the given channel, and W_α is the corresponding energy. Factors of the form $(W_n^{(0)} - W_\alpha)$ also appear in the higher-order terms of the perturbative expansion represented by the ellipsis.

As long as L is such that $W_\alpha = M_R$ is far from the free two-pion energy, $W_n^{(0)}$, all of the terms in the perturbative series are regular and can therefore be resummed. Now, if the resonance is narrow, the coupling of the resonance to the n_0, $\pi\pi$ state will be small. In turn, this means that the matrix element $\langle\pi\pi|H_{int}|R\rangle$ is small compared to the mass and typical energies of the system. [15] Moreover, the leading correction which the resonance brings to the interacting two-pion energy, W_n, appears at second order in the expansion. Thus, it is of order $|\langle\pi\pi|H_{int}|R\rangle|^2$ and is therefore small.

When $L = L_R$ such that $W_n^{(0)}(L_R) = M_R$, the effect of the resonance is radically different. Its second and higher order contributions to W_n blow up. In such a situation,

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[15] We assume here that the narrowness of the resonance is not only due to phase-space suppression.
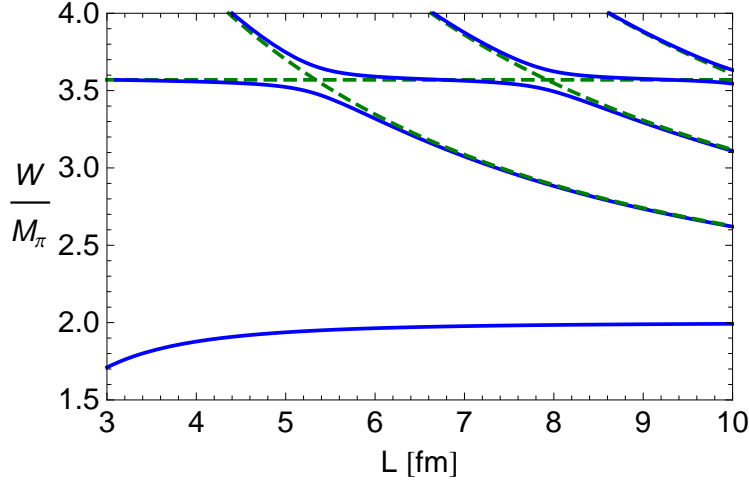
Fig. 3.3 The two-pion spectrum in a box of volume L^3 as a function of L in the $I = J = 0$ channel with an additional, fictitious resonance of mass $M_R = M_{K_S}$ and width $\Gamma_R = 10^{12} \times (\Gamma_{+-} + \Gamma_{00} - (4/3)\Gamma_{+0}) \simeq 7.3\,\text{MeV}$ with Γ_{+-}, Γ_{00}, and Γ_{+0} given in Eqs. (3.102)–(3.104). The dashed green curves represent the two-pion spectrum interacting through δ_0 (they correspond to the solid blue curves in Fig. 3.2). The solid blue curves show the interacting spectrum as obtained from Eq. (3.121), with the contribution of the resonance to the phase shift. At the points at which the resonance (i.e. the horizontal green dashed curve at $M_{K_S}/M_\pi \sim 3.57$) crosses the excited $I = J = 0$ states, one clearly sees a level repulsion effect. The effect is rather small and limited to a smallish region around the crossing point because the resonance is narrow: $\Gamma_R/M_R \simeq 1.5\%$.

we have to resort to degenerate perturbation theory and first diagonalize H in the two-state subspace $\{|n_0\rangle, |R\rangle\}$. This means diagonalizing the 2×2 matrix

$$\begin{pmatrix} \langle n_0|H|n_0\rangle & \langle n_0|H|R\rangle \\ \langle R|H|n_0\rangle & \langle R|H|R\rangle \end{pmatrix} = \begin{pmatrix} M_R & M_n \\ M_n^* & M_R \end{pmatrix} , \tag{3.128}$$

where $M_n \equiv \langle n_0|H|R\rangle$ is the transition amplitude between the resonance and the two-pion state $|n_0\rangle$. A straightforward diagonalization yields

$$W_n^{\pm} = M_R \pm |M_n| , \tag{3.129}$$

thereby lifting the degeneracy and giving rise to a typical level repulsion phenomenon. Thus, in solving Martin's formula (3.121), we would find a dependence of the two-pion energy as a function of L, which looks like what is depicted in Fig. 3.3.

3.11 $K \to \pi\pi$ **in finite volume**

What Martin and I realized over ten years ago is that to study $K \to \pi\pi$ decays in finite volume, we could treat the kaon as an infinitesimally narrow resonance in the

weak interaction contribution to the scattering of the two pions (Lellouch and Lüscher, 2001). In that case, one considers the free Hamiltonian to be the QCD Hamiltonian, i.e.

$$H_0 = H_{\text{QCD}} \ , \tag{3.130}$$

and the perturbation, H_{int}, to be the effective weak Hamiltonian relevant for $K \to \pi\pi$ decays, i.e.

$$H_{int} = H_W = \int_{x_0=0} d^3x \ \mathcal{H}_W(x) \ . \tag{3.131}$$

Then, since the amplitudes for $K \to \pi\pi$ decays, $T(K \to \pi\pi)$, are computed at $O(G_F)$, we can perform all of our computations to that order.

Following what was done in the preceding section for the resonance, we tune the size of the box to $L = L_K$, such that for some level n,

$$W_n(L_K) = M_K \ . \tag{3.132}$$

In that case, the corresponding pion momentum is the momentum, k_π, which the pions would have in the physical kaon decay, i.e.

$$k_n(L_K) = k_\pi \equiv \sqrt{\frac{M_K^2}{4} - M_\pi^2} \ . \tag{3.133}$$

Then, the transition matrix element in the finite volume $V = L_K^3$,

$$M_n^I \equiv {}_V\langle(\pi\pi)_I n|H_W|K\rangle_V \ , \tag{3.134}$$

is an energy conserving matrix element. Since finite-volume corrections to a single, stable particle state are exponentially small in L and since we neglect such corrections here, $|K\rangle_V$ is identical to $|K\rangle$, up to a purely kinematic normalization factor.

However, we are not interested in the finite-volume matrix element of Eq. (3.134). What we want is the infinite-volume transition amplitude,

$$T_I \equiv \langle(\pi\pi)_I n, out|\mathcal{H}_W|K\rangle \ , \tag{3.135}$$

where the corresponding A_I of Eq. (3.3) can be made real in the CP conserving case.

Because it is important here, let us pause to say a few words about the normalization of states used. In finite volume we use the usual quantum mechanical normalization of states to unity. Thus, for a spinless particle of mass m and momentum $\vec{p}$:

$$_V\langle\vec{p}|\vec{p}'\rangle_V = \delta_{\vec{p},\vec{p}'} \ . \tag{3.136}$$

In infinite volume, it is the standard relativistic normalization of states, i.e.

$$\langle p|p'\rangle = 2p^0(2\pi)^3\delta^{(3)}(\vec{p} - \vec{p}') \ , \tag{3.137}$$

with $p^0 = \sqrt{m^2 + \vec{p}^2}$, which is implemented.

To obtain the relationship between these two amplitudes, we compute the shift in energy brought about by the presence of the weak interactions in two different ways, and require the two results to agree.
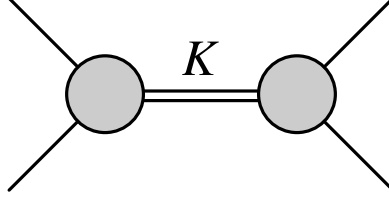
Fig. 3.4 Kaon contribution to the elastic weak scattering of two pions in the S-channel. The shaded vertices represent the $K \to \pi\pi$ transition amplitudes at $O(G_F)$.

We begin by repeating the degenerate perturbation theory of the preceding section. We obtain

$$W_n^\pm = M_K \pm |M_n^I| \, , \tag{3.138}$$

where M_n^I is clearly $O(G_F)$. Then, we turn to Martin's finite-volume quantization formula (3.121). In the presence of the weak interaction, the phase shift receives a weak contribution, δ_W. Thus, in that formula, we have to perform the replacement

$$\delta_I \to \bar{\delta}_I = \delta_I + \delta_W \, . \tag{3.139}$$

We are interested in this phase shift at the values of momenta $k = k_n^\pm$, corresponding to the perturbed energies $W_n^\pm$ of Eq. (3.138):

$$k_n^\pm = k_n \pm \Delta k = k_n \pm \frac{W_n |M_n^I|}{4k_n} + O(G_F^2) \, . \tag{3.140}$$

Indeed, we know that those values must come out of the quantization formula because the two methods of determining the energy shifts must give the same result. Because $W_n^\pm$ are "infinitesimally" close to M_K (in our LO counting in G_F), $\delta_W(k_n^\pm)$ is dominated by the s-channel kaon exchange depicted in Fig. 3.4. Any other contribution will be at least $O(G_F^2)$. In the s-channel, however, the factor of G_F^2 coming from the two K-$\pi\pi$ vertices is compensated by a propagator enhancement, due to the fact that we are sitting only $O(G_F)$ away from the peak of the resonance. Indeed, the scattering amplitude corresponding to Fig. 3.4 is

$$S[\text{Fig. 3.4}] = -\frac{\overbrace{T_I^* T_I}^{O(G_F^2)}}{\underbrace{(W_n^\pm)^2 - M_K^2}_{O(G_F)} - iM_K \underbrace{\Gamma_K}_{O(G_F^2)}} + O(G_F^2) \tag{3.141}$$

$$= \mp \frac{|A_I|^2}{2W_n^{(0)}|M_n^I|} + O(G_F^2) \, , \tag{3.142}$$

where we have used the fact that the vertices in Fig. 3.4 are the on-shell transition amplitudes up to higher order corrections in G_F. To translate this amplitude into a

scattering phase, we use the partial wave decomposition of a $\pi\pi$ scattering amplitude S in the center of mass frame: [16]

$$S = 16\pi\, W \sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta)\, e^{i\delta_l^I(k)}\, \frac{\sin\delta_l^I(k)}{k}\ , \qquad (3.143)$$

where $W = 2\sqrt{M_\pi^2 + k^2}$ is the energy of the pion pair. Since the amplitude of Eq. (3.141) has no angular dependence, it only leads to a zero angular momentum phase shift, which is the weak phase shift of interest. Thus, we find

$$\delta_W(k_n^\pm) = \mp \frac{k_n^\pm |A_I|^2}{32\pi (W_n^{(0)})^2 |M_n^I|} + O(G_F^2)\ . \qquad (3.144)$$

We can now include this contribution into the total phase shift $\bar{\delta}_I$ and write down the resulting quantization equation:

$$n\pi - \delta_I(k_n \pm \Delta k) \pm \frac{k_n^\pm |A_I|^2}{32\pi (W_n^{(0)})^2 |M_n^I|} = \phi(q_n \pm \Delta q) + O(G_F^2)\ , \qquad (3.145)$$

with $\Delta q = L\Delta k/(2\pi)$. Expanding this equation to $O(G_F)$, we finally find the relationship between the desired, infinite-volume amplitude A_I and the finite-volume matrix elements M_n^I, computed on the lattice (Lellouch and Lüscher, 2001):

$$|A_I|^2 = 8\pi \left\{ q\frac{\partial}{\partial q}\phi(q) + k\frac{\partial}{\partial k}\delta_I(k) \right\}_{k=k_n} \frac{(W_n^{(0)})^2 M_K}{k_n^3} L^6 |\mathcal{M}_n^I|^2\ , \qquad (3.146)$$

were we have used the definition

$$\mathcal{M}_n^I \equiv {}_V\langle (\pi\pi)_I n|\mathcal{H}_W(0)|K\rangle_V = M_n^I/L^3\ . \qquad (3.147)$$

In our derivation we have tuned the size of the box to L_K such that $W_n^{(0)} = M_K$ and thus, $k_n = k_\pi$ (Eqs. (3.132)–(3.133)). However, Eq. (3.146) is also valid for $W_n^{(0)} \neq M_K$, as can be seen in Sec. 3.12 and as was derived using the fact that the matching factor is related to the density of interacting two-pion states in finite volume (Lin *et al.*, 2001). An interesting discussion of this and other ways of looking at this formula is given in (Testa, 2005). In (Kim *et al.*, 2005), Eq. (3.146) was further generalized to moving frames, i.e. frames in which the center of mass has a nonvanishing momentum. And in (Kim and Sachrajda, 2010), it is shown how partially-twisted boundary conditions can be used to obtain the phase shift $\delta_2(k)$ and its derivative in the isospin-2 channel. With twisted boundary conditions, one allows some of the quark flavors to be periodic only up to a phase. This phase forces the flavors concerned to carry a momentum which is proportional to the phase. The boundary conditions are called partially-twisted when it is only the valence flavors which are given a twist.

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[16]Note that δ_l^I's subscript in Eq. (3.143) corresponds to angular momentum l, while the superscript is the isospin I. This notation will be used in this equation only. Elsewhere, δ's subscript will be the isospin, except for δ_W where W stands for weak.

The proportionality factor (3.146) is to a large extent kinematic, as it accounts for the difference in normalization of states in finite and infinite volumes, given in Eqs. (3.136)–(3.137). This can easily be seen in the absence of interactions. To reach the nth two-pion with energy $W_n^{(0)}$ and pion momentum $k_n^{(0)}$, the cube must have sides

$$L_n = \frac{2\pi}{k_n^{(0)}} \sqrt{n} \ . \tag{3.148}$$

Then, Eq. (3.146) assumes the form

$$|A_I|^2 = \frac{4}{\nu_n} (W_n^{(0)})^2 M_K L^3 |M_n^I|^2 \tag{3.149}$$

where

$$\nu_n \equiv \text{number of } \vec{z} \in \mathbb{Z}^3 \ \ni \ \vec{z}^2 = n \ . \tag{3.150}$$

The proportionality constant is precisely the relative normalization of free kaon and two-pion states in finite and infinite volume projected onto the A_1^+ and spin-0 sectors, respectively (see also Sec. 3.12). The constant is the product of the ratio of squared norms of the kaon state, $2M_K L^3$, and of the two-pion state, $2(W_n L^3)^2$, [17] times the square of the factor relating H_W and $\mathcal{H}_W(0)$, i.e. $1/L^6$, times $1/\nu_n$ since the finite-volume, A_1^+ state is obtained by summing over the ν_n pion momentum directions.

3.12 $K \to \pi\pi$ in finite volume: a simple relativistic quantum field theory example

To understand how the finite-volume effects predicted by Eqs. (3.121)–(3.146) show up in correlation functions similar to those one would use in numerical simulations, it is useful to consider them in the context of a relativistic field theory in which all quantities of interest can be computed analytically. Because the form of the finite-volume formulae (3.121) and (3.146) does not depend on the details of the dynamics, we choose to work in a world in which this dynamics is simplified, so as not to obscure the discussion of finite-volume effects with superfluous technical details. The calculations below were summarized in (Lellouch and Lüscher, 2001).

3.12.1 Specification of the model

We consider a theory of a single, neutral, spinless pion field $\pi(x)$, of mass M_π. In the notation of Sec. 3.11, the unperturbed Hamiltonian density is

$$\mathcal{H}_0 = \mathcal{H}_{\text{kin}} + \mathcal{H}_S \ , \tag{3.151}$$

where $\mathcal{H}_{\text{kin}}$ is the usual kinetic Hamiltonian of a scalar field and the "strong" interaction between the pions is given by

$$\mathcal{H}_S = \frac{\lambda}{4!} \pi^4 \ . \tag{3.152}$$

We assume here that the theory is perturbative in λ and we will work to first nontrivial order in λ, i.e. $O(\lambda)$. Because the lattice calculations are performed in Euclidean

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[17]The factor of 2 is required because the two pions in the final state are identical particles in the isospin limit which we consider here.

spacetime, we rotate this theory into the Euclidean and consider Euclidean correlation functions. Moreover, our calculations will be performed in a three-volume L^3 with periodic boundary conditions, but the time direction will be considered of infinite extent.

To make the perturbation theory completely well-defined, we introduce a Pauli-Villars cutoff Λ. At tree level the Euclidean pion propagator is then given by

$$S_\pi(x) = \int_x e^{ik \cdot x} \langle \pi(x)\pi(0) \rangle = \frac{1}{p^2 + M_\pi^2} - \frac{1}{p^2 + \Lambda^2} \ . \tag{3.153}$$

The cutoff should be large enough so that ghost particles cannot be produced at energies below the four-pion threshold, but in view of the universality of Eq. (3.121) and (3.146) there is no need to take Λ to infinity at the end of the calculation.

Since we are going to be computing correlation functions in the time-momentum representation, it is useful to have the pion propagator in this same representation. We have

$$S_\pi(t; \vec{k}) \equiv \int_{\vec{x}} e^{-i\vec{k} \cdot \vec{x}} \langle \pi(t, \vec{x})\pi(0) \rangle$$

$$= \frac{1}{2E_k} e^{-E_k |t|} - \frac{1}{2\mathcal{E}_k} e^{-\mathcal{E}_k |t|} \ , \tag{3.154}$$

where $E_k = \sqrt{\vec{k}^2 + M_\pi^2}$ and $\mathcal{E}_k = \sqrt{\vec{k}^2 + \Lambda^2}$.

As far as the kaon and its decays into two pions are concerned, the least complicated possibility is to describe it by a free hermitian field $K(x)$ with mass M_K and to take

$$\mathcal{H}_W = \frac{g}{2} K\pi^2 \tag{3.155}$$

as a weak Hamiltonian density. We will only work here to leading order in the weak coupling, also.

3.12.2 Determination of the phase shift

Let us first determine the phase shift, $\delta(k)$, in the model of Eq. (3.152). This is an infinite-volume, Minkowski space calculation, though at the order at which we work this fact makes very little difference. The partial wave decomposition of the invariant, scattering amplitude S, in the center-of-mass frame, is given in Eq. (3.143). At $\mathcal{O}(\lambda)$, $S = -\lambda$, and therefore

$$\delta(k) = -\frac{\lambda}{16\pi} \frac{k}{W} + O(\lambda^2) \ , \tag{3.156}$$

where $W = 2E_k$ is the free two-pion energy.

3.12.3 Two-pion energies using Eq. (3.121)

In the absence of interactions, i.e. for $\delta(k) \equiv 0$, the solutions of Eq. (3.121), for $n = 1, 2, \ldots, 6$, are the free, finite-volume momentum magnitudes, $k_n^{(0)} \equiv \sqrt{n}(2\pi/L)$. [18]

---

[18]Here and in the following, quantities with the superscript (0) are computed at $O(\lambda^0)$, while those without a superscript are the same quantities in the presence of the "strong" interaction of Eq. (3.152).

For weakly interacting pions, the solutions are small perturbations about these values. Thus, the rescaled momenta are

$$q_n = \frac{k_n L}{2\pi} = q_n^{(0)} + \Delta q_n = \sqrt{n} + \Delta q_n \; , \tag{3.157}$$

where Δq_n is the small perturbation.

To first order in Δq_n and λ

$$\tan \phi(q_n) = \frac{4\pi^2}{\nu_n} n \Delta q_n + \mathcal{O}(\Delta q_n^2) \; , \tag{3.158}$$

and Eq. (3.121) yields

$$\Delta q_n = \lambda \frac{\nu_n}{32\pi^2 \sqrt{n}} \frac{1}{W_n^{(0)} L} + \mathcal{O}(\lambda^2) \; , \tag{3.159}$$

where $W_n^{(0)} = 2\sqrt{M_\pi^2 + (k_n^{(0)})^2}$ is the energy of two free pions with opposite momenta of magnitude $k_n^{(0)}$. Thus, the energy of the corresponding two-pion state, in the presence of interactions, is

$$W_n = W_n^{(0)} \left(1 + \lambda \frac{\nu_n}{2} \frac{1}{(W_n^{(0)} L)^3} + \mathcal{O}(\lambda^2) \right) \; . \tag{3.160}$$

3.12.4   Two-pion energies from perturbation theory

In perturbation theory, the two-pion energy corresponding to pions whose momenta would have magnitude $k_n^{(0)}$, $n = 1, \ldots, 6$, in the absence of interactions, can be extracted from the $\pi\pi \to \pi\pi$ correlation function

$$C_{\pi\pi \to \pi\pi}(t) = \langle \mathcal{O}_n(t) \mathcal{O}_n(0) \rangle_{\mathrm{conn}} \; , \tag{3.161}$$

where

$$\mathcal{O}_n(t) = \frac{1}{\nu_n} \sum_{\{\vec{k}_n\}} \int_{\vec{x_1} \vec{x_2}} e^{i\vec{k}_n \cdot (\vec{x_2} - \vec{x_1})} \pi(t, \vec{x_2}) \pi(t, \vec{x_1}) \tag{3.162}$$

is an operator which has overlap with zero-momentum, cubically invariant, two-pion states and ν_n is the number of momenta $\vec{k}_n$ such that $|\vec{k}_n| = k_n^{(0)}$ (see Eq. (3.150)). The sum in Eq. (3.162) is over these momenta, all related by cubic transformations. The operator $\pi(x)$ has overlap with single pion states. In the limit of large t, the contribution of the two-pion states, $|\pi\pi \, l\rangle_V$, to the correlation function of Eq. (3.161), is

$$C_{\pi\pi \to \pi\pi}(t) \longrightarrow \sum_{l=0}^{6} |\langle 0 | \mathcal{O}_n(0) | \pi\pi \, l \rangle_V|^2 \, e^{-W_l t} + \cdots \; , \tag{3.163}$$

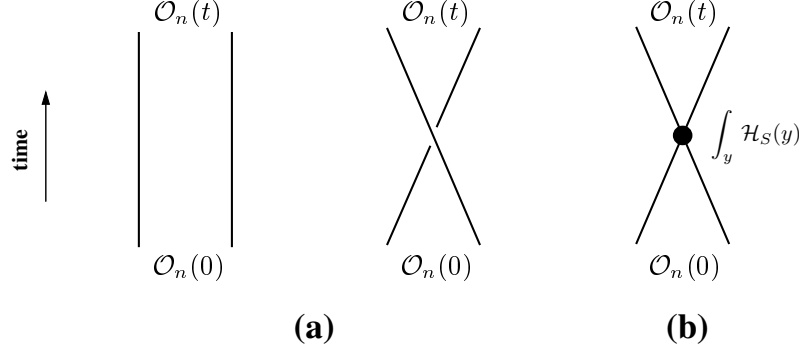where the ellipsis stands for terms which decay more rapidly. The states $|\pi\pi \, l\rangle_V$ are normalized to one.

Fig. 3.5 Diagrams which contribute to $C_{\pi\pi \to \pi\pi}(t)$ at $\mathcal{O}(\lambda^0)$ (a) and $\mathcal{O}(\lambda)$ (b).

A straightforward calculation of the diagrams of Fig. 3.5, using the propagator of Eq. (3.154), gives for the correlation function of Eq. (3.161), at $\mathcal{O}(\lambda)$,

$$C_{\pi\pi \to \pi\pi}(t)|_n = \frac{2}{\nu_n} \left(\frac{L^3}{W_n^{(0)}} \right)^2 e^{-W_n^{(0)}t} \left\{ 1 - \lambda \frac{\nu_n}{2L^3} \left(\frac{t}{(W_n^{(0)})^2} - \frac{1}{(W_n^{(0)})^3} \right. \right.$$

$$\left. \left. - \frac{R_\Lambda \left((k_n^{(0)})^2, (k_n^{(0)})^2 \right)}{2} \right) + \mathcal{O}(\lambda^2) \right\} \tag{3.164}$$

$$= \frac{2}{\nu_n} \left(\frac{L^3}{W_n} \right)^2 e^{-W_n t} \left\{ 1 + \lambda \frac{\nu_n}{2L^3} \left(\frac{1}{(W_n^{(0)})^3} + \frac{R_\Lambda \left((k_n^{(0)})^2, (k_n^{(0)})^2 \right)}{2} \right) + \mathcal{O}(\lambda^2) \right\} \ ,$$

where we have only retained the contribution which decays exponentially with the rate corresponding that of the two-pion state, $|\pi\pi\, n\rangle_V$. In Eq. (3.164), the two-pion energy, W_n, is the same as that obtained from the finite-volume formula of (Lüscher, 1991) (see Eq. (3.160)) and the regulator contribution is given by

$$R_\Lambda \left(\vec{p}^2, \vec{k}^2 \right) = \frac{4(E_p + \mathcal{E}_p)}{E_p \mathcal{E}_p \left[(E_p + \mathcal{E}_p)^2 - 4E_k^2 \right]} - \frac{1}{\mathcal{E}_p(E_p^2 - \mathcal{E}_p^2)} \ , \tag{3.165}$$

with self-explanatory notation.

Comparison of this result with Eq. (3.163) further gives the matrix element of $\mathcal{O}_n$ between the vacuum and the two-pion state, $|\pi\pi\, n\rangle_V$:

$$|\langle 0|\mathcal{O}_n(0)|\pi\pi\, n\rangle_V| = \sqrt{\frac{2}{\nu_n}} \left(\frac{L^3}{W_n} \right) \left\{ 1 + \lambda \frac{\nu_n}{4L^3} \left[\frac{1}{(W_n^{(0)})^3} + \frac{R_\Lambda \left((k_n^{(0)})^2, (k_n^{(0)})^2 \right)}{2} \right] \right.$$

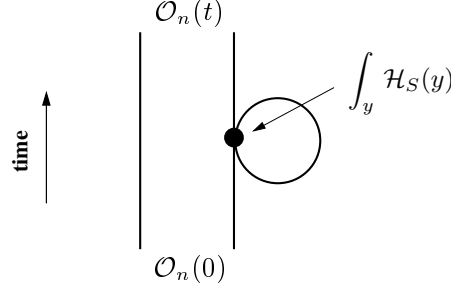$$\left. + \mathcal{O}(\lambda^2) \right\} \ . \tag{3.166}$$

Fig. 3.6 Example of a tadpole contribution to $C_{\pi\pi \to \pi\pi}(t)$ at $\mathcal{O}(\lambda)$.

The observant reader will have noticed that we have not taken into account contributions from diagrams such as the one of Fig. 3.6, which also appear at $\mathcal{O}(\lambda)$. As can be verified explicitly, these diagrams amount to a shift of the pion mass by terms which are independent of L, up to exponentially small corrections. Since such corrections are neglected here, these contributions will affect none of our finite-volume results, once the mass has been appropriately renormalized in infinite volume. The details of this renormalization are irrelevant here and we assume that the renormalization has been adequately performed. Furthermore, the coupling λ and the field $\pi(x)$ only get renormalized at $O(\lambda^2)$, which is beyond the order at which we are working.

3.12.5   Matching of finite to infinite matrix elements using Eq. (3.146)

Here we consider a weak transition between the state of a kaon at rest and a two-pion state, $|\pi\pi \, n\rangle_V$, in finite volume. The amplitude for this transition is

$$M = \int_{\vec{x}} {}_V\langle \pi\pi \, n | \mathcal{H}_W(0, \vec{x}) | K \rangle_V \; . \tag{3.167}$$

The corresponding infinite-volume transition amplitude, T, is given by

$$T = \langle \pi(\vec{p})\pi(-\vec{p}), out | \mathcal{H}_W(0) | K(\vec{0}) \rangle \; . \tag{3.168}$$

Again, infinite-volume states are relativistically normalized here.

To compare with the perturbative results obtained below, we must compute the factor relating $|T|$ and $|M|$ in Eq. (3.146) to $O(\lambda)$. Using the expressions in Eqs. (3.157)–(3.159) for q_n, and after some algebra, we find

$$q_n \phi'(q_n) = \frac{4\pi^2 n^{3/2}}{\nu_n} \left\{ 1 + \frac{\lambda}{8\pi^2} \frac{1}{W_n^{(0)} L} \left[\frac{\nu_n}{n} + z_n \right] + O(\lambda^2) \right\} \; , \tag{3.169}$$

where z_n is the constant given by

$$z_n = \lim_{q^2 \to n} \left\{ \sqrt{4\pi} \mathcal{Z}_{00}(1; q^2) + \frac{\nu_n}{q^2 - n} \right\} \; . \tag{3.170}$$

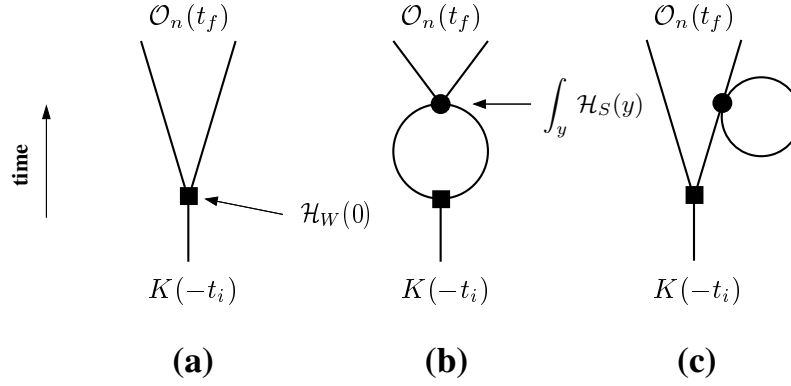Now, using the result of Eq. (3.156) for $\delta(k)$ and Eqs. (3.157)–(3.159) for k_n, we find

Fig. 3.7 Diagrams which contribute to $C_{K \to \pi\pi}(t_i, t_f)$ at $O(\lambda^0)$ (a) and $O(\lambda)$ (b,c).

$$k_n \delta'(k_n) = -\frac{\lambda}{8} \frac{\sqrt{n}}{W_n L} \left[1 - n \left(\frac{4\pi}{W_n^{(0)} L} \right)^2 + O(\lambda^2) \right] . \qquad (3.171)$$

Combining Eqs. (3.169)–(3.171), we find for the factor which relates $|T|$ and $|M|$ in Eq. (3.146),

$$8\pi \left\{ q \frac{\partial \phi}{\partial q} + k \frac{\partial \delta_0}{\partial k} \right\}_{k_n} \frac{M_K W_n^2}{k_n^3} \qquad (3.172)$$

$$= \frac{4 M_K W_n^2 L^3}{\nu_n} \left\{ 1 + \frac{\lambda}{2} \frac{1}{W_n^{(0)} L} \left[\frac{z_n}{4\pi^2} + \frac{\nu_n}{(W_n^{(0)} L)^2} \right] + O(\lambda^2) \right\} ,$$

where we have used the expression for k_n obtained in Eq. (3.157) and (3.159). It should be remarked that, unless the pions interact strongly, the size of this factor is essentially determined by mismatches in the definitions of T and M and in the normalization of states in finite and infinite volume (see Eq. (3.149) and subsequent discussion).

3.12.6 Matching of finite to infinite matrix elements from perturbation theory

The relevant correlation function here is

$$C_{K \to \pi\pi}(t_i, t_f) = \int_{\vec{x}} \langle \mathcal{O}_n(t_f) \mathcal{H}_W(0) K(-t_i, \vec{x}) \rangle . \qquad (3.173)$$

At $O(\lambda^0)$, it is given by the diagram in Fig. 3.7.a. One trivially obtains,

$$C_{K \to \pi\pi}^{(3.7.a)}(t_i, t_f) \Big|_n = -g \frac{e^{-M_K t_i}}{2 M_K} \frac{e^{-W_n^{(0)} t_f}}{(W_n^{(0)})^2} . \qquad (3.174)$$

At $O(\lambda)$, the contribution from the diagram in Fig. 3.7.b gives, using the pion propagators defined in Eq. (3.154),

$$C_{K \to \pi\pi}^{(3.7.b)}(t_i, t_f) \Big|_n = \lambda \frac{g}{2} \frac{e^{-M_K t_i}}{2 M_K} \int_{t_y} \frac{1}{L^3} \sum_{\vec{p}} \{ S_\pi(t_y; \vec{p}) \}^2 \times \{ S_\pi(t_f - t_y; \vec{k}_n) \}^2$$

$$\longrightarrow - \left. C_{K\to\pi\pi}^{(3.7.a)}(t_i, t_f) \right|_n \times \lambda \left\{ \frac{\nu_n}{2L^3} \left(\frac{t}{(W_n^{(0)})^2} + \frac{1}{(W_n^{(0)})^3} - \frac{R_\Lambda \left((k_n^{(0)})^2, (k_n^{(0)})^2 \right)}{2} \right) \right.$$

$$\left. + \frac{1}{8} \mathcal{A}(k_n^{(0)}) \right\} , \qquad (3.175)$$

where

$$\mathcal{A}(k_n^{(0)}) = \frac{1}{L^3} \sum_{\vec{p}}{}' \left[\frac{1}{E_p(\vec{p}^2 - (k_n^{(0)})^2)} - R_\Lambda \left(\vec{p}^2, (k_n^{(0)})^2 \right) \right] , \qquad (3.176)$$

and where we have only kept, in the second line of Eq. (3.175), the terms in the momentum sum of the first line which fall off as $e^{-W_n^{(0)} t_f}$.

The sum in Eq. (3.176) is restricted to momenta $\vec{p}$ such that $|\vec{p}| \neq k_n^{(0)}$. To evaluate it, we use the asymptotic, large-volume expansion of (Lüscher, 1986). Up to terms that vanish more rapidly than any power of $1/L$, we find

$$\mathcal{A}(k_n^{(0)}) \sim I_1(k_n^{(0)}) + \frac{z_n}{2\pi^2 W_n^{(0)} L} + \frac{\nu_n}{L^3} \left[\frac{4}{(W_n^{(0)})^3} + R_\Lambda \left((k_n^{(0)})^2, (k_n^{(0)})^2 \right) \right] , \qquad (3.177)$$

where z_n is defined in Eq. (3.170). In Eq. (3.177), $I_1(k_n^{(0)})$ is the infinite-volume contribution:

$$I_1(k_n^{(0)}) = \int_{\vec{p}} \left\{ \frac{1}{E_p} \mathrm{Re} \left[\frac{1}{\vec{p}^2 - (k_n^{(0)})^2 - i\epsilon} \right] - R_\Lambda \left(\vec{p}^2, (k_n^{(0)})^2 \right) \right\} . \qquad (3.178)$$

As discussed following Eq. (3.166), tadpole diagrams such as the one of Fig. 3.7.c solely contribute to the renormalization of the mass of the corresponding leg and do not affect our finite-volume expressions.

Combining Eqs. (3.174), (3.175) and (3.177), we find, at $O(\lambda)$,

$$C_{K\to\pi\pi}(t_i, t_f; k_n^{(0)}) \longrightarrow -g \left\{ 1 - \frac{\lambda}{8} I_1(k_n^{(0)}) \right\} \frac{e^{-M_K t_i}}{2M_K} \frac{e^{-W_n t_f}}{W_n^2} \times \qquad (3.179)$$

$$\times \left\{ 1 - \frac{\lambda}{8} \left(\frac{z_n}{2\pi^2 W_n^{(0)} L} - \frac{\nu_n R_\Lambda \left((k_n^{(0)})^2, (k_n^{(0)})^2 \right)}{L^3} \right) + O(\lambda^2) \right\} ,$$

where, again, W_n, is given by Eq. (3.160).

3.12.7 Putting it all together

The contributions of the two-pion states, $|\pi\pi\, l\rangle_V$, to $C_{K\to\pi\pi}(t_i, t_f)$ are, in the limit of large t_i and t_f,

$$C_{K\to\pi\pi}(t_i, t_f) \longrightarrow \sum_{l=0}^{6} e^{-M_K t_i - W_l t_f} \langle 0 | \mathcal{O}_n(0) | \pi\pi\, l \rangle_V \; {}_V\langle \pi\pi\, l | \int_{\vec{x}} \mathcal{H}_W(0, \vec{x}) | K \rangle_V$$

$$\times\ _V\langle K|K(0)|0\rangle + \cdots , \tag{3.180}$$

where the ellipsis stands for terms which decay more rapidly. In Eq. (3.180), $|K\rangle_V$ is a zero-momentum state and, again, all states are normalized to 1. With these normalizations,

$$_V\langle K|K(0)|0\rangle = \sqrt{\frac{1}{2M_K L^3}} . \tag{3.181}$$

Combining this matrix element with Eqs. (3.179)–(3.180) and the result of Eq. (3.166) for $|\langle 0|\mathcal{O}_n(0)|\pi\pi\, n\rangle_V|$, we find

$$|M| = g\left\{1 - \frac{\lambda}{8}I_1(k_n^{(0)})\right\}\frac{1}{2}\sqrt{\frac{\nu_n}{M_K W_n^2 L^3}}\left\{1 - \frac{\lambda}{4}\frac{1}{W_n^{(0)}L}\left[\frac{z_n}{4\pi^2} + \frac{\nu_n}{(W_n^{(0)}L)^2}\right]\right.$$
$$\left. + O(\lambda^2)\right\} , \tag{3.182}$$

Now, a straightforward evaluation of the infinite-volume analogs of the diagrams of Fig. 3.7 yields:

$$T = -g\left\{1 - \frac{\lambda}{8}\int_{\vec{p}}\left[\frac{1}{E_p(\vec{p}^2 - (k_n^{(0)})^2 - i\epsilon)} - R_\Lambda\left(\vec{p}^2, (k_n^{(0)})^2\right)\right]\right\} . \tag{3.183}$$

Therefore,

$$\frac{|T|}{|M|} = 2\sqrt{\frac{M_K W_n^2 L^3}{\nu_n}}\left\{1 + \frac{\lambda}{4}\frac{1}{W_n^{(0)}L}\left[\frac{z_n}{4\pi^2} + \frac{\nu_n}{(W_n^{(0)}L)^2}\right] + O(\lambda^2)\right\} , \tag{3.184}$$

which is in perfect agreement with the result of Eq. (3.172), predicted by the finite-volume formula of Eq. (3.146). In obtaining Eq. (3.184), we have used the fact that $|T| = |\mathrm{Re}\,T| + O(\lambda^2)$.

3.12.8 $K \to \pi\pi$ in finite volume: physical kaon decays

For illustration, let us suppose that the S-wave scattering phases δ_I, $I = 0, 2$, are accurately described by the one-loop formulae of chiral perturbation theory (Gasser and Meissner, 1991; Knecht *et al.*, 1995). The two-pion energy spectrum can then be calculated in the isospin I channel and in a box of size L where level $n = 1$ coincides with the kaon mass. With this input, the proportionality factor in Eq. (3.146) is easily evaluated and one ends up with (cf. Table 3.1)

$$|A_0| = 44.9 \times |M_0|, \tag{3.185}$$
$$|A_2| = 48.7 \times |M_2|, \tag{3.186}$$
$$|A_0/A_2| = 0.92 \times |M_0/M_2|. \tag{3.187}$$

As these results show, the large difference between the scattering phases in the two isospin channels (about 45° at $k = k_\pi$) does not lead to a big variation in the proportionality factors. In fact, if we set the scattering phases to zero altogether, Eqs. (3.148)–(3.149) give $|A_I| = 47.7 \times |M_I|$ for $n = 1$, which is not far from the results quoted

I	L [fm]	q	$q\partial\phi/\partial q$	$k\partial\delta_I/\partial k$
0	5.34	0.89	4.70	1.12
2	6.09	1.02	6.93	-0.09

Table 3.1 Calculation of the proportionality factor in Eq. (3.146) at the first level crossing

above. This may be surprising at first sight, since the interactions of the pions in the spin and isospin 0 state are quite strong. However, one should take into account the fact that the comparison is made for box sizes L which are greater than 5 fm. Hence, it is quite plausible that the finite-volume matrix elements already include most of the final-state interaction effects. Apart from a purely kinematic factor, only a small correction is then required to obtain the infinite-volume matrix elements, from the finite-volume ones.

The proportionality factor in Eq. (3.146) thus appears to be only weakly dependent on the final-state interactions. In particular, if the theory is to reproduce the $\Delta I = 1/2$ enhancement, the large factor has to come from the ratio of the finite-volume matrix elements M_I. In fact, if you carry out this calculation, you should see an 8% enhanced $\Delta I = 1/2$ enhancement!

To carry out this calculation you will have to address a couple of issues which have not yet been discussed here. The first is that, in the absence of twisted boundary conditions, at least the first excited $\pi\pi$ energy will have to be extracted from the lattice calculation, This requires cross-correlator techniques constructed from operators such as the one given in Eq. (3.162) and solving the resulting generalized eigenvalue problem (GEVP), as described in (Lüscher and Wolff, 1990). The second issue is the one of the renormalization of the lattice matrix elements. This is an important, but fairly technical problem, which depends sensitively on the fermion discretization used. It is usually referred to as the *ultraviolet* problem, as opposed to the *infrared* problem which we dealt with here, which is associated with the continuation of the theory to Euclidean spacetime and the use of a finite volume in numerical simulations. Unfortunately I will not have the time to cover the ultraviolet problem here. This problem has been studied quite extensively, and I refer you to the original literature, as well as to the lectures of Peter (Weisz, 2010) and Tassos (Vladikas, 2010) in this volume. For Wilson fermions, which explicitly break chiral symmetry, but retain a full flavor symmetry, the problem has been studied in the following series of papers (Bochicchio *et al.*, 1985; Maiani *et al.*, 1987; Bernard *et al.*, 1988; Dawson *et al.*, 1998). For twisted-mass QCD, the reference is (Frezzotti and Rossi, 2004). When considering domain-wall fermions with a finite fifth dimension, one should follow the renormalization set forth for Wilson fermions. However, for domain-wall fermions the required subtractions should be significantly smaller, since the chiral symmetry breaking should be significantly suppressed compared to what it is for Wilson fermions. Regarding discretizations which have the full, continuum chiral-flavor symmetry at finite lattice spacing (e.g. overlap fermions, or domain-wall fermions with a practically infinite fifth dimension), the renormalization is much simplified and will proceed as in the continuum. Finally, for staggered fermions, these issues are discussed in (Sharpe *et al.*, 1987; Sharpe and Patel, 1994).

To conclude, if you wish to be the first particle theorist to unambiguously see the $\Delta I = 1/2$ rule in $K \to \pi\pi$ decays and determine ϵ' with controlled errors, I hope that you begun working on the problem immediately after the course was given. If not, you would do better to hurry because the RBC-UKQCD collaboration is making quick progress on these problems (Christ, 2010a; Liu, 2010; Sachrajda, 2010b).

4

Appendix: integral representation for $Z_{00}(1; q^2)$

Here we derive an integral representation for the zeta function $Z_{00}(1; q^2)$ of Eq. (3.123), which is a meromorphic function of q^2, with poles at $q^2 = \vec{n}^2$, $\vec{n} \in \mathbb{Z}^3$. This representation is particularly effective for evaluating numerically the kinematic function $\phi(q)$ that appears in Martin's two-particle momentum quantization formula Eq. (3.121). It differs from the one given in Appendix C of (Lüscher, 1991).

The definition of $Z_{00}(s; q^2)$ is given by Eq. (3.123):

$$Z_{00}(s; q^2) = \frac{1}{\sqrt{4\pi}} \sum_{\vec{n} \in \mathbb{Z}^3} \left(\vec{n}^2 - q^2 \right)^{-s} .$$

We define

$$Z_{00}^{>\Lambda}(s; q^2) = \frac{1}{\sqrt{4\pi}} \sum_{\vec{n}^2 > \Lambda} \left(\vec{n}^2 - q^2 \right)^{-s} , \tag{4.1}$$

where the sum runs over all $\vec{n} \in \mathbb{Z}^3$ such that $\vec{n}^2 > \Lambda$ with $\Lambda \geq \operatorname{Re} q^2$. For $\operatorname{Re} s > 0$,

$$Z_{00}^{>\Lambda}(s; q^2) = \frac{1}{\Gamma(s)} \sum_{\vec{n}^2 > \Lambda} \int_0^\infty dt\, t^{s-1}\, e^{-t(\vec{n}^2 - q^2)}$$

$$= \frac{1}{\Gamma(s)} \sum_{\vec{n} \in \mathbb{Z}^3} \int_0^1 dt\, t^{s-1}\, e^{-t(\vec{n}^2 - q^2)} + \Delta(s; q^2) , \tag{4.2}$$

with

$$\Delta(s; q^2) = \frac{1}{\Gamma(s)} \left\{ \sum_{\vec{n}^2 > \Lambda} \int_1^\infty dt - \sum_{\vec{n}^2 \leq \Lambda} \int_0^1 dt \right\} t^{s-1}\, e^{-t(\vec{n}^2 - q^2)} , \tag{4.3}$$

where the second sum runs over all $\vec{n} \in \mathbb{Z}^3$ such that $\vec{n}^2 \leq \Lambda$.

To evaluate the sum in Eq. (4.2), we use a Dirac comb:

$$\sum_{\vec{n} \in \mathbb{Z}^3} f(\vec{n}) = \sum_{\vec{n} \in \mathbb{Z}^3} \int d^3x\, f(\vec{x})\, \delta^{(3)}(\vec{x} - \vec{n})$$

$$= \sum_{\vec{n} \in \mathbb{Z}^3} \int d^3x\, f(\vec{x})\, e^{i2\pi \vec{n} \cdot \vec{x}} . \tag{4.4}$$

With $f(\vec{n}) = e^{-t\vec{n}^2}$ and

$$\int_{-\infty}^{+\infty} dx\, e^{-tx^2 + i2\pi nx} = \sqrt{\frac{\pi}{t}} e^{-\frac{\pi^2 n^2}{t}} \,, \tag{4.5}$$

Eq. (4.4) yields

$$\sum_{\vec{n} \in \mathbb{Z}^3} e^{-t\vec{n}^2} = \sum_{\vec{n} \in \mathbb{Z}^3} \left(\frac{\pi}{t}\right)^{3/2} e^{-\frac{\pi^2 \vec{n}^2}{t}} \,. \tag{4.6}$$

Thus

$$Z_{00}^{>\Lambda}(s; q^2) = \frac{1}{\Gamma(s)} \sum_{\vec{n} \in \mathbb{Z}^3} I(s; \vec{n}) + \Delta(s; q^2) \,, \tag{4.7}$$

with

$$I(s; \vec{n}) = \pi^{3/2} \int_0^1 dt\, t^{s-5/2} e^{tq^2 - \frac{\pi^2 \vec{n}^2}{t}} \,. \tag{4.8}$$

Viewed as a function of $\vec{n}$, $I(s; \vec{n})$ is singular only for $\vec{n} = \vec{0}$ when $\mathrm{Re}\, s \leq 3/2$. In that case, I's integrand goes like $t^{s-1-3/2}(1 + tq^2 + O(t^2))$ when $t \to 0$. Thus, $\mathrm{Re}\, s > 3/2$ yields the half-plane in complex s for which the expression of Eq. (4.7) gives a finite result. For such s we can write

$$I(s; \vec{0}) = \pi^{3/2} \int_0^1 dt\, t^{s-5/2} \left(e^{tq^2} - 1\right) + \frac{\pi^{3/2}}{s - 3/2} \,, \tag{4.9}$$

which is actually well defined for $\mathrm{Re}\, s > 1/2$ and $s \neq 3/2$. Thus, for all s in the half plane $\mathrm{Re}\, s > 1/2$, we obtain

$$\sqrt{4\pi} Z_{00}(s; q^2) = \sum_{\vec{n}^2 \leq \Lambda} (\vec{n}^2 - q^2)^{-s} + \frac{\pi^{3/2}}{\Gamma(s)} \left\{ \frac{1}{s - 3/2} + \int_0^1 dt\, t^{s-5/2}(e^{tq^2} - 1) \right.$$

$$\left. + \sum_{\vec{n}^2 \neq 0} \int_0^1 dt\, t^{s-5/2} e^{tq^2 - \frac{\pi^2 \vec{n}^2}{t}} \right\} + \Delta(s; q^2) \,, \tag{4.10}$$

where the last runs over all $\vec{n} \in \mathbb{Z}^3$ such that $\vec{n}^2 \neq 0$.

Now, for the case $s = 1$ which is of interest to us here, it is straightforward to compute $\Delta(s; q^2)$:

$$\Delta(1; q^2) = \left\{ \sum_{\vec{n}^2 > \Lambda} \int_1^\infty dt - \sum_{\vec{n}^2 \leq \Lambda} \int_0^1 dt \right\} e^{-t(\vec{n}^2 - q^2)}$$

$$= \sum_{\vec{n}^2 > \Lambda} \frac{e^{-(\vec{n}^2 - q^2)}}{\vec{n}^2 - q^2} + \sum_{\vec{n}^2 \leq \Lambda} \frac{e^{-(\vec{n}^2 - q^2)} - 1}{\vec{n}^2 - q^2} \,. \tag{4.11}$$

Using this result in the expression of Eq. (4.10) for $Z_{00}(s; q^2)$ with $s = 1$, we obtain:

$$Z_{00}(1; q^2) = -\pi + \frac{1}{\sqrt{4\pi}} \sum_{\vec{n} \in \mathbb{Z}^3} \frac{e^{-(\vec{n}-q^2)}}{\vec{n} - q^2} + \frac{\pi}{2} \int_0^1 \frac{dt}{t^{3/2}} (e^{tq^2} - 1)$$

$$+ \frac{\pi}{2} \sum_{\vec{n} \neq \vec{0}} \int_0^1 \frac{dt}{t^{3/2}} e^{tq^2 - \frac{\pi^2 \vec{n}}{t}}$$

$$= -\pi + \frac{1}{\sqrt{4\pi}} \sum_{m=0}^{\infty} \nu_m \frac{e^{-(m-q^2)}}{m - q^2} + \frac{\pi}{2} \int_0^1 \frac{dt}{t^{3/2}} (e^{tq^2} - 1)$$

$$+ \frac{\pi}{2} \sum_{m=1}^{\infty} \nu_m \int_0^1 \frac{dt}{t^{3/2}} e^{tq^2 - \frac{\pi^2 m}{t}} \quad , \tag{4.12}$$

where ν_m counts the $\vec{n} \in \mathbb{Z}^3$ such that $\vec{n}^2 = m$ (see Eq. (3.150)). Eq. (4.12) is the integral representation that we were after. Using this representation, it is straightforward to calculate $Z_{00}(1; q^2)$ numerically with good efficiency and high precision, using standard integration routines.

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